PREDICTION OF COKE QUALITY AND COKE RATE USING FUZZY-LOGIC AND GENETIC ALGORITHMS

by

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DEPARTMENT OF MATERIALS AND METALLURGICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

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PREDICTION OF COKE QUALITY AND COKE RATE USING FUZZY-LOGIC AND GENETIC ALGORITHMS

A Thesis Submitted

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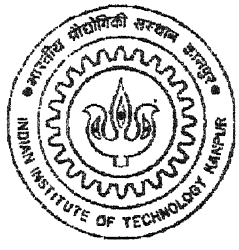
by

PUNYA SHEEL



to the

DEPARTMENT OF MATERIALS AND METALLURGICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

MAY, 1999

CERTIFICATE

It is certified that the work contained in this thesis entitled **Prediction of Coke Quality and Coke Rate Using Fuzzy Logic and Genetic Algorithms** has been carried out by **Mr. Punya Sheel** under my supervision and that this work has not been submitted elsewhere for the award of a degree.

Brahma Deo 5.5.99

Dr. Brahma Deo

Professor and Head,

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Indian Institute of Technology, Kanpur.

कर्मण्येवाधिकारस्ते मा फलेषु कदाचन।
मा कर्मफलहेतुर्भूर् मा ते संगोऽस्त्वकर्मणि।।४७।।

अध्याय २: गीता

–to my beloved *Dadiji* & *Naniji*,

Mummy, Papa, Bawa

and

Diddle.

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People who made my stay at IIT Kanpur enjoyable and miserable at times.

I and my friends at IITK (I could not get a group photograph)

... ASaiKumar ASateeshKumar AbhishekNigam AlokThapar AmritaMukhrjee Anant-Mishra AnubhavManglik AnujVyas ArvindKumarRajput AshishSrivastva Ashutosh-Gopinath AtulKumarDobhal AvinashJha BharatVirSingh BhushanDhutkar BijayBhu-jbal CGopiKrishna CRajakartikeyan ChanderPrakash DSridharSastry DeveshKishore DinniLingraj DiwakarRathode GaneshPrabhakarKulkarni&Sadhana GopeshAggarwal HimanshuKSingh IVRao JramaKrishna KapilGupta KhemChandJoshi KshitizKrishna KulbirSingh LRamakrishna **PunySheel** MahendraUmranikar ManojChaudhary ManojSharma MilanBarui Mohd.Farhan Mr&MrsAnupKumar Mr&MrsManishPande Murali MurtuzaD NBabu NahasMYahiya NandKishorePrasad Navneet NihalChand-Jain NitinSanghi PPhaniKumar PSambaSivaRaju PSurendraKumar ParathaSarthiDe PiyushKumar PranayKumarSwain PrasadLimaye PratulSharma PraveenVyas RCRa-maswamy RahulShukla RajeevDutta RajeevGupta RajeevKumar RamSharanSingh RameshSharma SKTomar SanjayMishra SanjeevSharma SanjitAnand SankhaGhosh SantoshBMalge SantoshSingh SarabjitDutta SauravJindal ShaileshTiwari SharadA-grawal ShishirSihna SiddarthMukherjee SomanshuJend SomnathBanerjee Sriram-Murthy SumeetGupta VRajesh VaibhavJain VijayMisra VikrantJain VinayJohar Vi-neetJain

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PUNYA SHEEL

Contents

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List of Symbols

$\{\}$	Parabolic penalty
$\langle\rangle$	Bracket operator penalty
$A, B, C,$ $D, E, F,$ G, H, I	Constants in empirical relation developed to predict stability
$A_1, A_2, \ldots, A_n$	Coefficients in the regression model equation
$\widetilde{A_i}$	ith fuzzy coefficients in the fuzzy regression model equation
B	net burden rate ($kilogram/Metric Ton of Hot Metal\,(MTHM)$)
$C_1, C_2, \ldots, C_6$	Constants in empirical coke rate equation
c	constant term in regression line equation
c_i	Spread of ith fuzzy number
E	Measure of coke economy (%)
E_b	Kinetic energy of the blast
$F(x)$	Mathematical function in x
$f(x)$	Mathematical function in x

$g_j(x)$	jth inequality constraint function in x
HV	High volatile coal
h	Some constant ($0.0 \leq h \leq 1.0$)
$h_k(x)$	kth equality constraint function in x
i	V-type
K	Coke rate ($kg/MTHM$)
K_i	*Strength Index* for ith V-type
L	Large
LM	Large Medium
LV	Low volatile coal
M	Medium
ML	Medium Large
MS	Medium Small
MV	Medium volatile coal
m	Slope of regression line
N	Total number of population
Obj	Objective function to be maximized or minimized
P	Absolute blast pressure (atm)
Pr	Productivity or hot metal production rate ($MTHM$)

P^*	Pellet percentage of gross burden
p_i	Mid-point or center-point of ith fuzzy number
Q	Driving rate or coke burned $(MetricTon/day)$
R	Correlation coefficient
R^2	Coefficient of determination
R_i	Reactives percentage of ith V-type
R^*	Set of penalty parameters
r	Lowest order V-type
S	Small
S_r	Sinter percentage of gross burden
s	Highest order V-type
SM	Small Medium
T	Blast temperature (K)
T_0	Theoretical flame temperature in front of tuyers before increasing the blast temperature $(°C)$
T_0'	Theoretical flame temperature in front of tuyers after increasing the blast temperature $(°C)$
t	Generation number
V	Blast volume $(Nm^3/second)$

V_i	ith V-type
V_{type}	V-type
VL	Very Large
VLM	Very Large Medium
VVL	Very Very Large
VS	Very Small
VSM	Very Small Medium
VVS	Very Very Large
$w_0, w_1, \ldots w_3$	Weights in the artificial neural network model
x	independent variable in regression model equation
x_i	ith variable in x
x_i^L	Lower bound of ith variable x
x_i^U	Upper bound of ith variable x
y	Dependent variable in the regression model equation
$\tilde{y}$	Fuzzy dependent variable in a fuzzy regression model equation

Greek Symbols

α	Constant used in defining bracket operator penalty
μ_y	Membership function of a fuzzy number y

σ	Standard error of estimation
σ^*	Sigmoidal function
ω	Penalty term

Abstract

Coal is an important raw material for ironmaking. Coal from different sources exhibit different rheological, chemical and petrographic properties. For an efficient blast furnace operation it is imperative that all the above properties of coal are simultaneously satisfied. However, a coal from a particular source does not fulfill all the necessary requirements. Therefore there is an effort on the part of ironmaker to blend coals from various sources to achieve a (*i*) low ash content, (*ii*) low sulfur content, (*iii*) low alkali content, (*iv*) high coke strength after reaction (CSR) and (*v*) high stability at a minimum cost. In the process of finding properties like predicted stability and CSR, the empirical curves suggested in literature were digitalized. Fuzzy associative memory (FAM) - a new technique has been used in curve fitting. In the first part of the present work coal samples from six different sources with known properties (mentioned above) have been considered and the most suitable blend combination has been arrived at by using an optimization technique - Genetic Algorithms (GA).

The second part of the thesis deals with the coke rate prediction in the blast furnace. Coke consumption rate (or coke rate) is a direct reflection of the hot metal production rate of a blast furnace. As the coke rate is decreased the blast furnace hot metal production increases. Operating plant parameters affecting the coke rate are hot blast temperature ($^{\circ}C$), cold blast flow (Nm^3), blast pressure (atm) , slag rate ($kg/MTHM$), top pressure (atm), hot metal production (MT), sinter rate ($kg/MTHM$), iron ore ($kg/MTHM$) and limestone consumption (MT). Actual plant data from Visakhapatnam Steel Plant, Visakhapatnam, India, collected over a period of six months has been used in developing coke rate prediction models. Various modeling techniques such as (*i*) multiple linear regression, (*ii*) stepwise linear regression, (*iii*) non-linear regression using neural network, (*iv*) fuzzy regression using linear programming, (*v*) fuzzy-GA regression and (*vi*) normal regression using GA, to predict coke rate have been employed and a comparative study carried out. Fuzzy-GA regression is a new technique developed in this work. Fuzzy-GA regression model proved to be the best of the modeling techniques exhibiting a very high correlation coefficient (for both $y = mx$ and $y = mx + c$ plots correlation coefficient was 0.9999) and low standard deviation (for $y = mx$ plot $\pm 0.40\, kg/MTHM$ and for $y = mx + c$ plot $\pm 0.395\, kg/MTHM$).

Chapter 1

Introduction

1.1 Introduction

Coke being the chief source of heat, is a very important raw material in the production of iron in the blast furnace. It also provides bed permeability and produces the reducing gases which play an important role in the blast furnace during iron making. It is produced in coke ovens from coal by the process of coking. Coal thus affects the quality and characteristics of coke produced. More uniformity is there in the properties of coal the better coke is produced and better is the quality of iron thus produced.

Coal that comes to steel plant is procured from different sources. Generally, the coals with different properties and different costs are mixed so as to get a low cost blend for the plant processing. Present work is devoted to two aspects; optimization of coal blend and prediction of coke rate in the blast furnace. In the part I of this thesis the aim is to optimize the properties of the coal blend at lowest cost to the steel producer. Also, the properties of the blend should be within acceptable limits; for example, coke strength after reaction should be minimum 61.0, predicted stability

should greater than 50.0, ash content of blend should not exceed 9.0% whereas the total sulfur should not be more than 0.82%. Also, another blend requirement to be met is that it should have high volatile coals (40 – 70%), medium volatile coals (10 – 40%) and low volatile coals (10 – 35%). Details of quality requirements are further discussed in section 4.2.

Maximum production of hot metal at the lowest cost is the prime objective of the ironmaker. To achieve this an important factor is coke requirement per unit ton of hot metal produced. In part II of the thesis, the effect of various parameters affecting coke rate are identified and various models have been developed to predict coke rate on the basis of different operating parameters. A new technique of modeling, named "fuzzy-GA regression" modeling has been developed in the present work and found to be very successful.

1.2 Thesis Organization

This thesis is divided into two parts. The first part covers the coal optimization for getting an optimum blend of coke and the second with the blast furnace coke rate prediction using a new technique developed in this work, fuzzy-GA regression.

Chapter 1. The current chapter, gives introduction to the work carried out in this Thesis.

Part I

Chapter 2. Chemical, rheological and petrographic properties of coal are discussed in this chapter. The properties like stability of coke and coke strength after reaction (CSR), moisture and ash content of coal are discussed here. The standards used to

determine these properties are also discussed.

Chapter 3. The Genetic Algorithms have been very briefly discussed here. Micro-GA (μGA) is also explained. The GAs are the optimizers used in this work.

Chapter 4. Problem formulation for optimizing with GA so as to get best blend compositions is discussed in this chapter.

Chapter 5. Techniques to model different prediction graphs is discussed in this chapter. This chapter contains the results obtained and discussion based on these results.

Part II

Chapter 6. The coke rate prediction in blast furnace, it's importance and parameters affecting it are discussed here. Also the plant data used for coke rate prediction is also given.

Chapter 7. Statistical method of regression to obtain relation models and different modeling techniques used in coke rate prediction, like artificial neural networks, fuzzy regression, etc. are described. A new regression technique based on "fuzzy-GA regression" which has been developed in the present work is discussed in detail.

Chapter 8. This chapter of the thesis contains results obtained from various models developed for coke rate prediction.

Chapter 9. Conclusions of Part I (Coke Blend Optimization) and Part II (Coke Rate Prediction) are summarized in this chapter.

Part I

Coal Blend Optimization

Chapter 2

Evaluation of Coal Properties

Rheological and chemical properties of coal like plastic range, ash content and sulfur decide the properties of coke. These coal properties and their testing methods are briefly described here.

2.1 Rheological Properties of Coal

2.1.1 Plastic Properties of Coal

The plastic range is the difference of the coal's softening temperature and solidification temperature. Mathematically, it can be represented as,

$$Plastic\,Range = Solidification\,Temperature - Softening\,Temperature \quad (2.1)$$

Constant Torque Gieselerr Plastometer measures the thermoplastic properties of coal by a standard method as described in ASTM D2639 [1][2]. The test involves packing of 5.0 g of coal (passing a $0.42mm$ sieve) around a metal stirring rod, called

a rabble arm in a vented metal crucible. A constant torque (calibrated to suspend $40g$) is applied to the stirrer when the crucible is immersed in a molten solder bath and brought to the thermal equilibrium around $300°C$. The temperature of crucible is then increased uniformly at $3.0°C/min$ and the rate of movement of the stirrer in dial-divisions-per-minute ($100\,divisions/360°\,rotation$) is measured in relation to the increase in temperature. Important values noted during test are:

1. The initial softening temperature of coal
2. The maximum fluid temperature recorded at maximum dial movement
3. The solidification temperature recorded when dial movement stops, and
4. The maximum fluidity or the maximum rate of dial movement.

The solidification and softening temperatures are then used to calculate the *Plastic Range* from equation 2.1.

2.2 Chemical Properties of Coal

The ultimate analysis is done to obtain the chemical composition of coal. The moisture, ash and volatile matter are the three values that are obtained by proximate analysis. The various testing methods to find the volatile matter, ash content, moisture and sulfur are discussed here briefly.

2.2.1 Volatile Matter

The volatile matter is represented as the percentage of gaseous products (excluding moisture) released from the coal under specific test conditions. The standard test method is ASTM D3175 [3] in which $1.0g$ of coal sample material is pulverized to

pass through $0.25mm$ sieve. The $-25mm$ fraction is weighed in a platinum crucible, covered with a closely fitting lid, and placed into a furnace maintained at a temperature of $950 \pm 20°C$ for exactly 7 minutes. No temperature fluctuation is permitted during testing. After heating the crucible is removed and cooled to room temperature and the observed loss in the weight of sample is used to calculate the percentage of volatile matter according to the equation 2.2 given below.

$$Volatile\ Matter(\%) = \left[\left\{\frac{(weight\ of\ sample - weight\ of\ residue}{weight\ of\ sample}\right\} \times 100\right] - Moisture(\%) \tag{2.2}$$

Several variations of test procedure exist depending upon the type of fuel viz. non-sparking coals, sparking, fuels and cokes.

2.2.2 Moisture and Ash

The moisture in coal is the percentage of uncombined water in the coal and ash is the percentage mass residue obtained after heating the coal sample under controlled conditions. The ASTM standards for moisture and ash are ASTM D3173 [3] and ASTM D3174 [3], respectively. The two analyses can be performed using the same sample and the results can be used for the proximate and ultimate analysis of coal. According to the ASTM procedure D3173 [3], $1.0g$ of $-0.25mm$ size coke is weighed into a pre-dried, tarred crucible and placed into a preheated moisture oven at a temperature between $104 - 110°C$ for one hour. The crucible is removed, covered and allowed to cool to room temperature in a dessicator. A final weight is recorded and is used to calculate percentage moisture with the following equation 2.3,

$$Moisture(\%) = \left[\frac{weight\ of\ sample - weight\ of\ residue}{weight\ of\ sample}\right] \times 100 \tag{2.3}$$

The moisture test sample may be used for determination of ash (following the standard D3174 [3]) by placing the uncovered crucible containing the sample in a cold furnace and heat gradually at such a rate that the temperature reaches $450-500°C$ in one hour. During heating there should be exchange of 2 to 4 volumes of air per minute moving through furnace. Heating of the sample is continued at a different rate so that within a second hour the temperature reaches $700-750°C$. Ashing is continued at this temperature for two additional hours, where upon the sample is removed, a cover is placed on crucible and cooled in a desiccator to room temperature. The final weight is recorded and the percentage ash is calculated from the equation 2.4,

$$Ash(\%) = \left[\frac{weight\,of\,(residue + container) - weight\,of\,container}{weight\,of\,dry\,sample\,used}\right] \times 100 \quad (2.4)$$

2.2.3 Total Sulfur

Sulfur content of coal is an important parameter in coal selection as high sulfur coals are not preferred. The standard for determining sulfur content of coal is ASTM D3177 [3] which includes two methods for determination of total sulfur, viz. Eschka Method and Bomb Washing Method.

- **Eschka Method**

  The coal sample is ignited in intimate contact with an Eschka mixture (i.e. 2 parts by weight light calcined MgO with 1 part anhydrous Na_2CO_3), the soluble sulfur compounds are leached out and oxidized to form sulphates, followed by acidification and precipitation as barium sulphate, which is filtered, ignited and weighed.

- **Bomb Washing Method**

Sulfur is precipitated as barium sulphate from oxygen-bomb calorimeter washings and the precipitate is filtered, ignited and weighed.

2.2.3.1 Sulfur Determination Using Combustion Methods

Sulfur determination by combustion methods (ASTM standard D4239 [3]) is done by three alternate procedures using high temperature tube furnace combustion methods for the rapid determination. These methods were designed to be used with the commercially available sulfur analyzers. Because sulfur values are empirically derived by these techniques/instruments, the apparatus must be calibrated by the use of standard reference materials (SRM) of known sulfur content. Briefly, the methods are summarized below:

- **Acid-base Titration Detection Procedure**

  A weighed sample is burned in a tube furnace at more than $1350°C$ in a stream of oxygen. During combustion, all sulfur is oxidized to gaseous sulfur oxides and the chlorine in the sample is released as Cl_2. The products are absorbed into a solution of H_2O_2, forming dilute H_2SO_4 and HCl acids. The quantity of acid is determined by titration, but to determine sulfur content a calibration with a SRM must be employed to correct for chlorine content.

- **Iodimetric Detection Procedure**

  A weighed sample is burned in a tube furnace at more than $1350°C$ in a stream of oxygen. The products are absorbed into aqueous solution containing iodine. When SO_2 is scrubbed by the diluent, the trace iodine is reduced to iodide, thus causing an increase in resistance across a polarized dual platinum electrode. Iodine titrant is then added proportionally to the solution until the excess iodine

is replenished and the solution resistance is reduced to its initial value. The volume of titrant consumed is used to calculate the sulfur concentration.

- **Infra-Red Absorption Detection Method**

  A sample is combusted in oxygen stream at temperature of $1350°C$ or above. Moisture and particulates are removed from the gas stream with traps and then passes through a cell in which sulfur-dioxide is measured by an infrared (IR) absorption detector. Sulphur-dioxide absorbs IR energy at a fixed wavelength, thus as energy is absorbed by gas stream, less energy is received at the detector. All other IR energy is eliminated before it reaches detector using filters. The absorption of IR energy can be attributed only to SO_2 whose concentration is proportional to the change in energy at the detector.

2.3 Petrographic Properties of Coal

The microscopic analysis of coal composition forms the basis for the study of petrographic properties of coal. The microscope reveals that coal is heterogeneous in composition. A polished coal surface when observed under a microscope can be subdivided into a number of discrete organic (maceral) and inorganic (mineral) constituents. Research has shown that the various macerals of coal react differently in coking process [4] and that sum total of these reactions is responsible for the coking behaviour of coal and the characteristics of the resulting coke.

The constituents of coal can be grouped into three broad categories. The first category is "reactives", which generate gas, soften, and become fluid before resolidifying into a bridging matrix that binds together the "inerts", (which constitute the second category) which do not appreciably change during coking. The third category "semi-inerts", have behaviour intermediate between those of reactives and inerts.

Coking potential of a coal or coal mix can be predicted from petrographic analysis provided the total reactives, the total inerts, and the kinds of reactions in a coal can be properly described and accurately quantified. It was also determined [5] that specific strength of the reactive binder is a function of the distribution of rank in the coal or coal blend and that this rank distribution[1] can be meaningfully quantified by measuring the reflectance of particles of the maceral vitrinite. The volume fraction of each coal constituent and the rank distribution of coal can be correlated with the results of carbonization tests, such as coke strength test as reported by Ammosov et al. [5] and Schapiro et al. [7]. These tests can be easily carried out on small samples in a short time. The kind of reactives are determined by reflectance analysis of the vitrinoids in a coal and these procedures have been discussed extensively in literature [8][9]. The vitrinoids, which appear as uniformly gray areas under the microscope, constitute the bulk of most coals and exercise major control over coking properties. The reflectance of vitrinoids increases as the rank of coal increases [4].

2.3.1 Stability of Coke

Stability of coke is a measure of abrasion resistance and it is defined as an index to determine the resistance to breakage and hardness at the room temperature. The stability should be high so that coke is sufficiently strong to withstand severe handling during it's movement.

U. S. Steel was the first to devise the coke stability prediction method based on tests conducted on several samples on eastern U. S. coals. It was found that at each given reflectance level there was an optimum inert content (ratio of reactives to

[1]Coals are classified according to the properties as defined by their rank (or degree of metamorphism), type(constituent plant material) and grade(degree of impurities and calorific value). Metamorphism is defined as the change in the structure of coal by natural agencies such as pressure or heat. Based on degree of metamorphism or rank, there are four classes of coals: anthracite, bituminous, sub-bituminous and lignite [6].

inerts) at which maximum coke strength was obtained. It was also found that at for a constant inerts (or reactives) content there was an optimum reflectance distribution at which the maximum coke strength occurred.

Coke strength, under specific coking conditions, is governed by two major factors:

- The relative amounts of inert and reactive macerals, and
- The strength of binding materials created when the reactive macerals are coked or carbonized.

U. S. Steel has developed a system for predicting coke stability from coal petrographic analyses by finding strength and inert constants for each level of vitrinite reflectance, called V-Types. The strength constants then can be used to calculate relative strength of binding material formed by the reactives, and inert constant can be used to calculate the effect of actual inert content relative to the optimum inerts for associated V-Types. The relative strength of the binding material was referred to as the "rank index" and relative effect of inerts as called "inert index" or "composition balance index". U. S. Steels has correlated these two indices with coke stability produced from pilot-scale coking tests and compiled the results in the form of iso-stability graph, as shown in Figure 2.1.

Researchers at Illinois State Geological Survey (ISGS) [10], however, found that the U. S. Steel method could not be applied to certain Illinois coals, or blends with these coals, and therefore produced their own stability prediction graph as shown in Figure 2.2.

Bethlehem Steel Corporation [11] researchers found that U. S. Steel method could not be used to predict stability for those coals which contained distinct maceral, which they called pseudovitrinite, and established a prediction method that took care

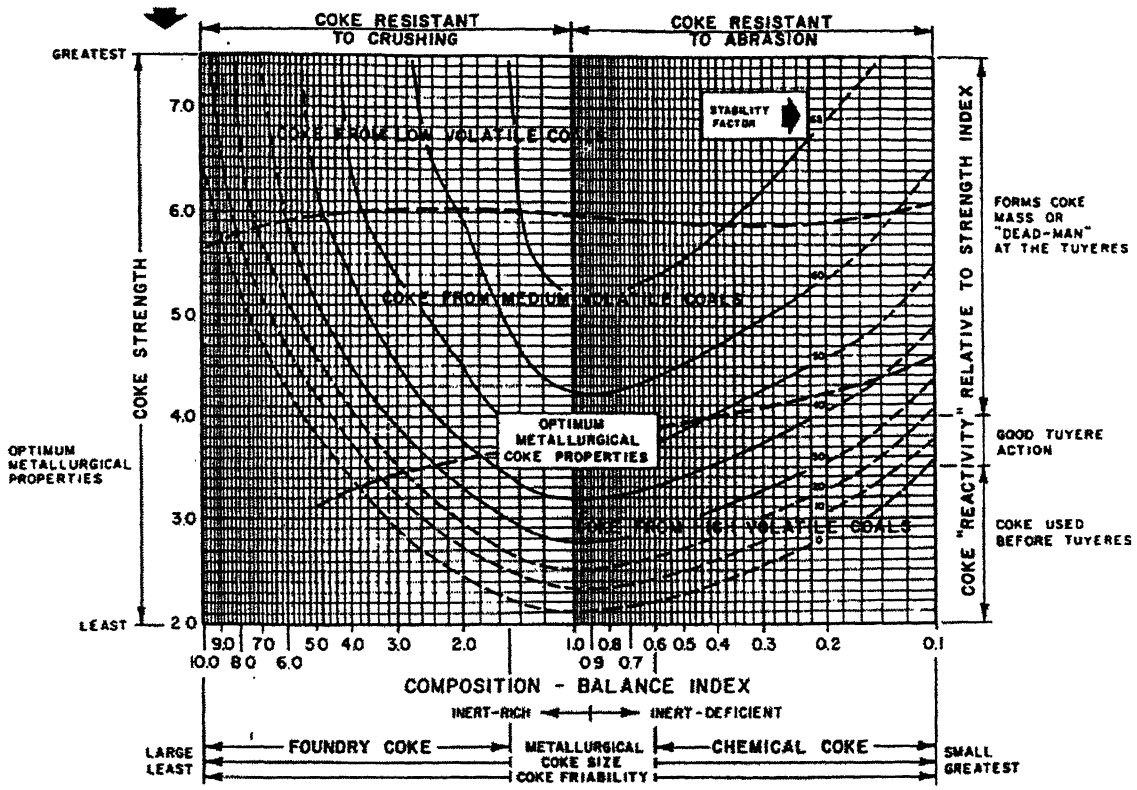


Figure 2.1: US Steel Stability Prediction Method

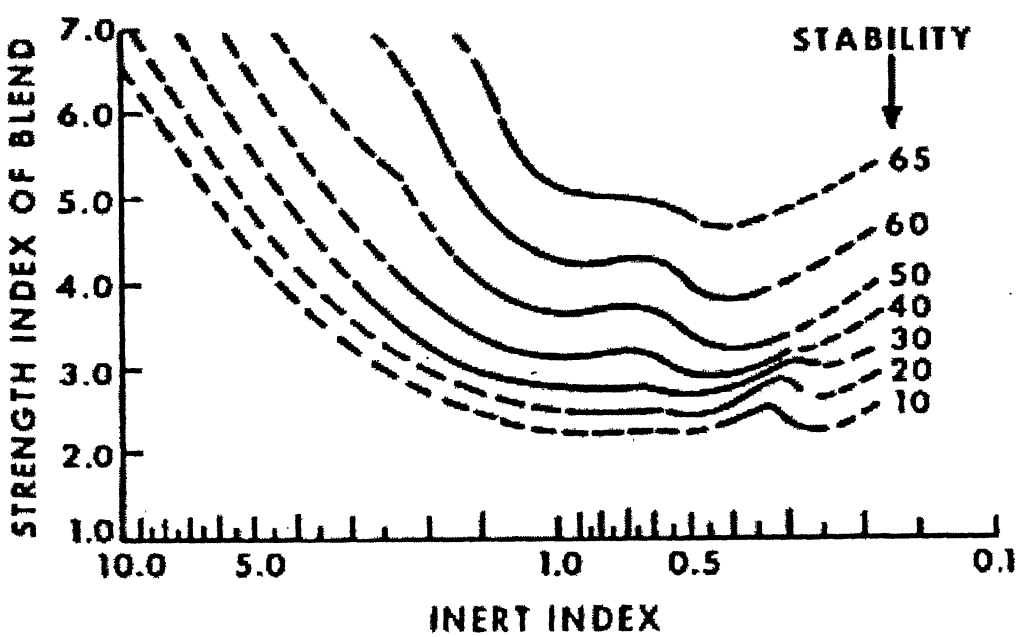


Figure 2.2: Illinois State Geological Survey (ISGS) Stability Prediction Graph

of pseudovitrinite effect. To avoid complication, they directly correlated stability to reflectance and inert content.

Another prediction method (unpublished) used by Consolidation Coal Company (Consol) [12] is a synthesis of U. S. Steel and ISGS methods and the resulting iso-stability graph is shown in Figure 2.3.

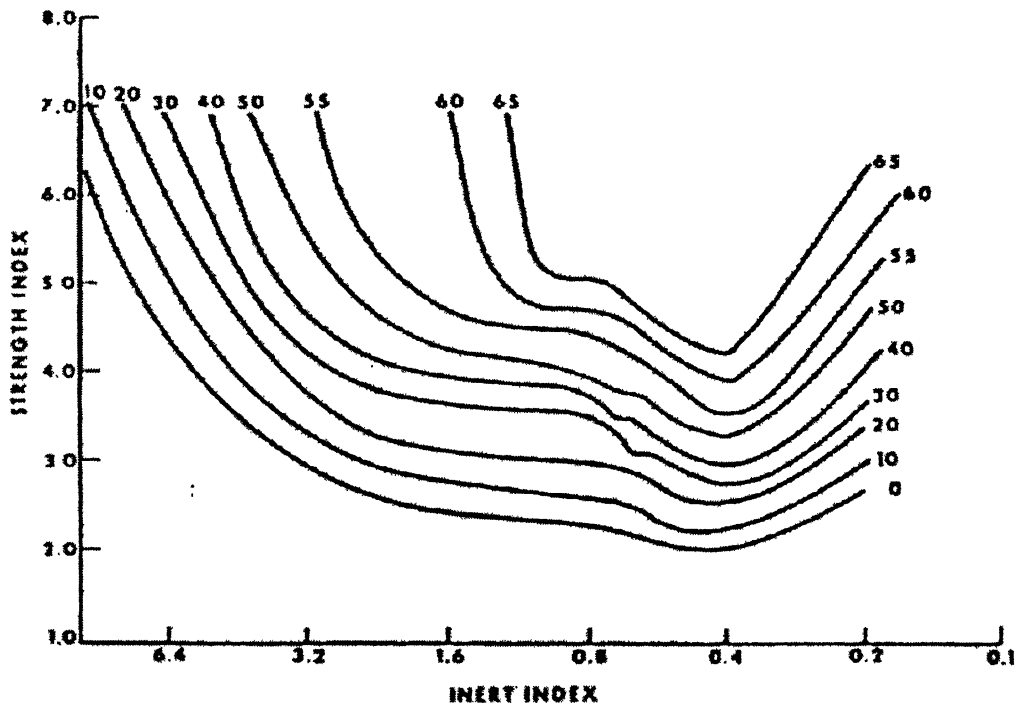


Figure 2.3: Consol Stability Prediction Graph

The method used in this work has been developed by the researchers at Inland Steel Research Laboratories. Coke stability for their coals could not be done satisfactorily by existing stability prediction methods. Hence they correlated rank and inert indices for strength and inert constants, and pseudovitrinite composition with coke stability as found in the coking tests. This was achieved by manually contouring actual coke stability as function of rank and inert indices. Also, most accurate stability predictions were accomplished by using strength and inert constants of Consol, as shown in Figure 2.4 and Figure 2.5, respectively; pseudovitrinite is considered to be

65.5% inert. For easy calculation, a factor of $\frac{2}{3}$ for inert and $\frac{1}{3}$ for reactive was used for all semifusinite, semimacrinite and also pseudovitrinite. The resulting correlation between coal composition indices and coke stability is shown in Figure 2.6.

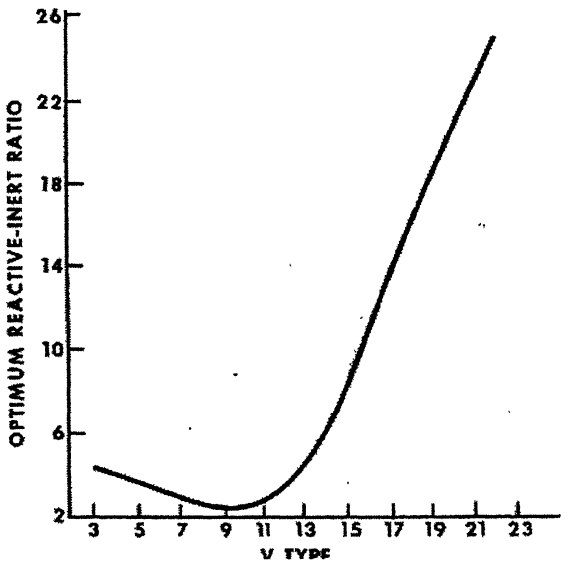


Figure 2.4: Optimum Reactive-Inert Ratio Graph

The data thus obtained can be used to predict the strength of coke produced by carbonization of single coals or coal blends. Companies also use coal petrography to design and improve coal preparation and coking equipment and to predict other coking factors as coke yield, wall pressure, coke reactivity, etc.

2.3.2 Prediction of Indices and Stability of Coke

Reflectance of Vitrinite is established for the purpose of determining the rank distribution of sample in terms of V-Types (reflectance increments of 0.1%) e.g., a vitrinite with reflectance of 0.69% would be classified as V-Type 6 (V6). Similarly that with reflectance of 0.81% would be classified as V-Type 8 (V8), and so on.

The maceral composition of the sample is determined for the purpose of calculating it's reactive and inert contents using the equations 2.5 and 2.6 respectively,

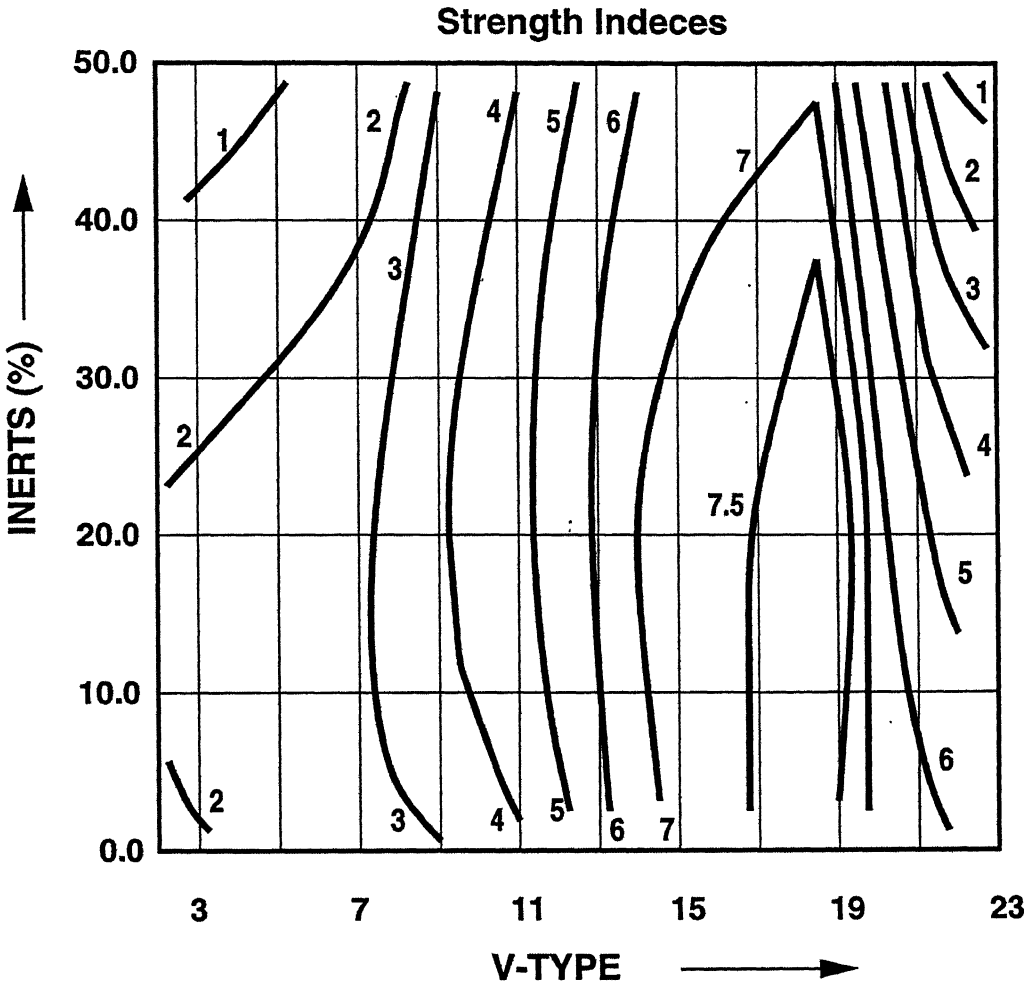


Figure 2.5: Strength Indices Chart

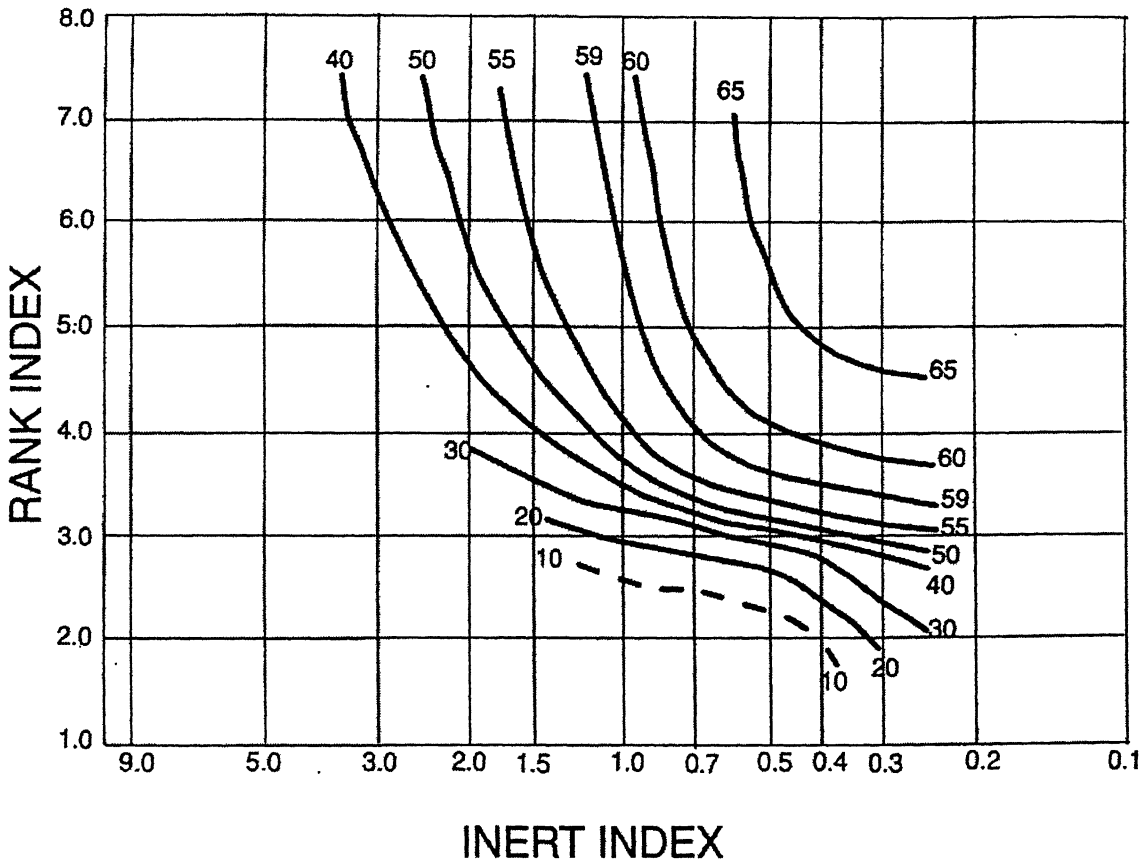


Figure 2.6: Stability Prediction Graph (Inland)

$$\%reactives = \left[\%vitrinite + \%exinite + \frac{1}{3}\{\%semifusinite\}\right] \times \frac{100}{sum} \quad (2.5)$$

$$sum = total\ of\ maceral\ composition\ including\ mineral\ matter$$

$$\%inerts = 100.0 - \%reactives \quad (2.6)$$

The *reactives* are prorated into V-Types according to the vitrinite reflectance distribution. Thus, if 20% of the vitrinite fell into V6, then the 20% of the reactive semifusinite, semimacrinite and pseudovitrinite would be treated as if it were vitrinite of category V6. This procedure results in all reactives being treated as vitrinite or vitrinite equivalents. The V-Type composition of the reactives is then used to calculate the optimum inerts for the sample. The *Optimum Inerts* is the percentage of inerts that the sample should contain to produce optimum coke stability for its rank distribution. It is calculated using equation 2.7,

$$Optimum\ Inerts = \sum_{i=r}^{s} \frac{R_i}{Optimum\ Ratio\ for\ V_i} \quad (2.7)$$

where,

i is the V-Type,

R_i is the percentage reactives in i,

r is the lowest order V-Type present,

s is the highest order V-Type present, and

Optimum Ratio for a particular V_i is obtained from Figure 2.4.

The *Inert Index* is then calculated by dividing the *Total Inerts* in the coal by the *Optimum Inerts*.

$$Inert\ Index = \frac{Total\ Inerts}{Optimum\ Inerts} \tag{2.8}$$

The *Rank Index* is obtained by first calculating the *Strength Index* of the reactives by,

$$Strength\ Index = \sum_{i=r}^{s} \frac{R_i}{K_i} \tag{2.9}$$

where,

i is the V-Type,

R_i is the percentage reactives in i,

r is the lowest order V-Type present,

s is the highest order V-Type present, and

K_i is the *Strength Index* for i as determined from Figure 2.5. The *Rank Index* is then calculated by dividing the *Strength Index* by the *Total Reactives* in the sample using equation 2.10.

$$Rank\ Index = \frac{Strength\ Index}{Total\ Reactives\ in\ Coal} \tag{2.10}$$

The predicted stability value can be obtained by applying the *Rank Index* and *Inert Index* to Figure 2.7.

2.3.2.1 Sample Calculation for Prediction of Indices and Stability for Single Coal

Sample Calculation for Maple Creek coal.

Mineral Matter in the coal is calculated from the amount of *Ash* and *Sulfur* present in the coal using Parr's formula. The amount of *Ash* and *Sulfur* is calculated

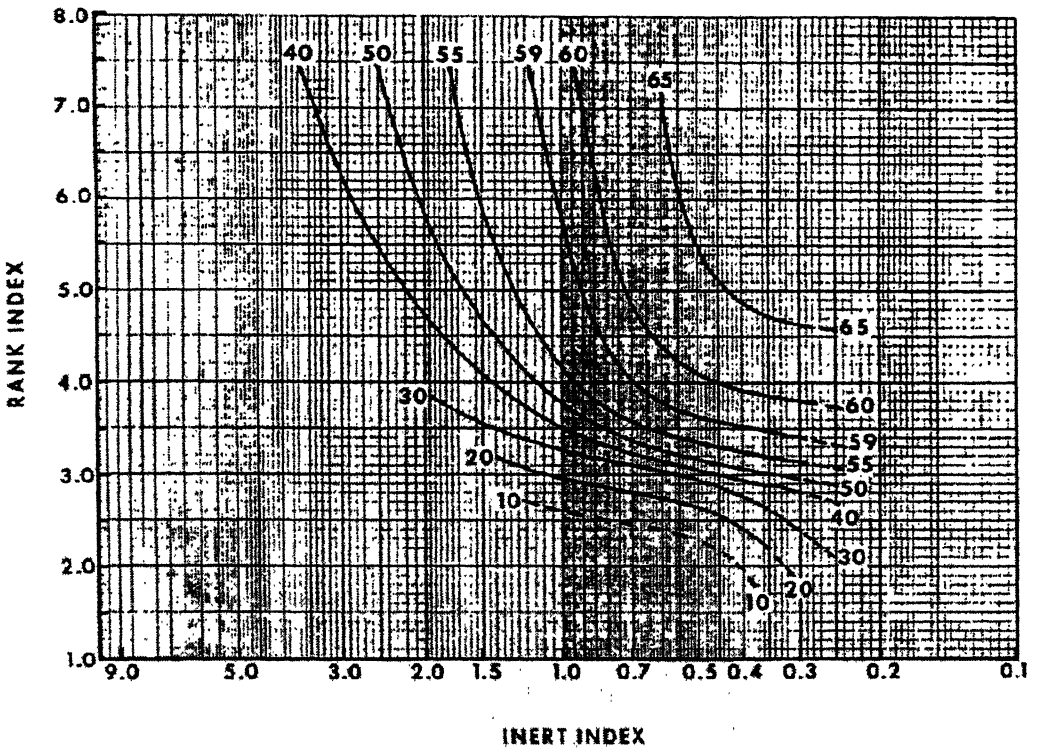


Figure 2.7: Predicted Stability from Inert Index and Rank Index

Table 2.1: Maceral Analysis for Sample Coal Maple Creek

Maceral	(%)
Vitrinite	84.60
Pseudovitrinite	0.00
Fusinite	5.60
Semifusinite	6.60
Macrenite	0.00
Semimacrinite	0.00
Micrinite	0.40
Oxyvitrinite	0.00
Exinite	2.80
Sum	100.00

from the chemical analysis. Actual Parr's formula is given below as equation ,

$$Mineral\ Matter = \left[\frac{\left[\frac{(1.08 \times Ash)+(0.55 \times Sulfur)}{2.8}\right] \times 100}{\left[\frac{100-\{(1.08 \times Ash)+(0.55 \times Sulfur)\}}{1.35}\right] + \left[\frac{(1.08 \times Ash)+(0.55 \times Sulfur)}{2.8}\right]} \right] \tag{2.11}$$

The formula given above in equation 2.11 can be approximated to,

$$Mineral\ Matter = \left[\frac{(1.08 \times Ash) + (0.55 \times Sulfur)}{2}\right] \tag{2.12}$$

If value of $Ash = 6.61\%$ and $Sulfur = 1.28\%$, using equation 2.12, we get,

$$\begin{aligned} Mineral\ Matter &= \left[\frac{(1.08 \times 6.61) + (0.55 \times 1.28)}{2}\right] \\ &= 3.92 \end{aligned}$$

The prorated maceral composition of coal with mineral matter is given is Table 2.2.

Table 2.2: Maceral Analysis with Mineral Matter for Coal Maple Creek

Maceral	(%)	Prorated (%)
Vitrinite	84.60	81.28
Pseudovitrinite	0.00	0.00
Fusinite	5.60	5.38
Semifusinite	6.60	6.34
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	0.40	0.38
Oxyvitrinite	0.00	0.00
Exinite	2.80	2.69
Mineral Matter	——	3.92
Sum	100.00	100.00

Table 2.3: Vitrinite Reflectance Distribution

V-Type	% of vitrinite	Prorated to % of coal
V7	4.00	4
V8	75.00	75
V9	21.00	21
Total	100.00	100

Using equations 2.5 and 2.6,

$$\begin{aligned} \%reactives &= \left[\%vitrinite + \%exinite + \frac{1}{3}\{\%semifusinite\}\right] \times \frac{100}{sum} \quad (2.13) \\ &= \left[81.28 + 2.69 + \frac{1}{3}\{6.34\}\right] \times \frac{100}{100.00} \\ \%reactives &= 86.09 \\ \%inerts &= 100.0 - \%reactives \quad (2.14) \\ &= 100.0 - 86.09 \\ \%inerts &= 13.91 \end{aligned}$$

Using vitrinite reflectance distribution from Table 2.3, reactives are prorated as V-Types,

$$\begin{aligned} \text{V7} &= 86.09 \times \tfrac{4}{100} = 3.44 \\ \text{V8} &= 86.09 \times \tfrac{75}{100} = 64.56 \\ \text{V9} &= 86.09 \times \tfrac{21}{100} = 18.08 \end{aligned}$$

from Figures 2.4 and 2.5 the optimum ratios and strength indices are obtained respectively, and are listed in Table 2.4,

From Table 2.4 substituting optimum ratios in equation 2.7 are used to get *Optimum Inerts* which are used further to get *Inert Index*.

Table 2.4: Optimum Ratios and Strength Indices for Corresponding V-Types

V-Type	Optimum Ratio	Strength Index
V7	3.0	3.0
V8	2.8	3.2
V9	2.6	3.5

$$\begin{aligned} Optimum\,Inerts &= \sum_{i=r}^{s} \frac{R_i}{Optimum\,Ratio\,for\,V_i} \\ &= \left[\frac{3.44}{3.0} + \frac{64.56}{2.8} + \frac{18.08}{2.6}\right] \\ &= 31.10 \end{aligned} \tag{2.15}$$

$$\begin{aligned} Inert\,Index &= \frac{Total\,Inerts}{Optimum\,Inerts} \\ &= \frac{13.91}{31.10} \\ &= 0.45 \end{aligned} \tag{2.16}$$

Using strength indices from Table 2.4 and equation 2.9, we get,

$$\begin{aligned} Strength\,Index &= \sum_{i=r}^{s} \frac{R_i}{K_i} \\ &= [(3.44 \times 3.0) + (64.56 \times 3.2) + (18.08 \times 3.5)] \\ &= 283.44 \end{aligned} \tag{2.17}$$

From equations 2.8 and 2.9 *Rank Index* can be calculated using equation 2.10,

$$\begin{aligned} Rank\ Index &= \frac{Strength\ Index}{Total\ Reactives\ in\ Coal} \\ &= \frac{283.44}{86.09} \\ &= 3.29 \end{aligned} \tag{2.18}$$

Predicted Stability can be read off from Figure 2.7,

$$Predicted\ Stability = 54.95$$

Data for all the six coals and the predicted stability is given in Appendix A. To summarize the predicted stbility indices are listed in Table below.

Table 2.5: Predicted Stability Indices of All Six Coals

Coal	Stability Index
Amburgy	49.69
Maben	41.87
Maple Creek	54.95
Riverside Sewell	59.02
Terry Eagle	59.29
Wells	58.37

2.3.3 Coke Strength After Reaction (CSR)

The coke strength after reaction (CSR) is essentially the resistance of coke to disintegrate under mechanical loading that occurs at high temperature in blast furnace. The use of coal petrography to predict blast furnace coke strength has previously been investigated by Kaegi [12]. Valia [13][14] has worked on CSR prediction using

CO_2. The CSR test was developed by Nippon Steel during 1970's. In this test, the coke is heated to $1100°C$ and placed in a constant stream of CO_2 gas for two hours. The coke is then cooled in an inert atmosphere and tumbled in an I-tumbler. Finally, it is screened through a $+10mm$ to calculate the CSR value.

2.3.3.1 CSR Prediction Methods

Various coal quality parameters in different combinations have been used by researchers for estimating CSR. Some of the methods are as follows:

2.3.3.1.1 NSC, Kobe Steel and British Steel Prediction Methods The CSR was correlated with reflectance and inertinite content of coal, as shown in Figure 2.8 [15]. CSR increases with increasing reflectance up to 1.40 percent reflectance. For each reflectance level, highest value of CSR is found at optimum inertinite value. Increase in inertinite beyond the optimum value or increase in coal reflectance beyond 1.40 percent decreases CSR. The correlation was however, not good (0.40) and the standard deviation was high (9.39) (see Figure 2.9). The prediction was poor because coals with high plastic properties or high alkali content were present. In the subsequent work, a factor called alkali index of coal ash was used by NSC researchers for CSR prediction; the alkali index is defined as the product of coal ash content times the ratio of mole fraction of $[CaO + MgO + Fe_2O_3 + Na_2O + K_2O]$ to $[SiO_2 + Al_2O_3]$.

Kobe Steel method differs from the NSC method with respect to larger top size coke samples, different temperature control procedures and shorter tumbling time of the reacted coke [16][17]. Kobe Steel refers coke strength after reaction with CO_2 as Reaction Strength Index (RSI). RSI is calculated on basis of mean reflectance, maximum fluidity and alkali content as,

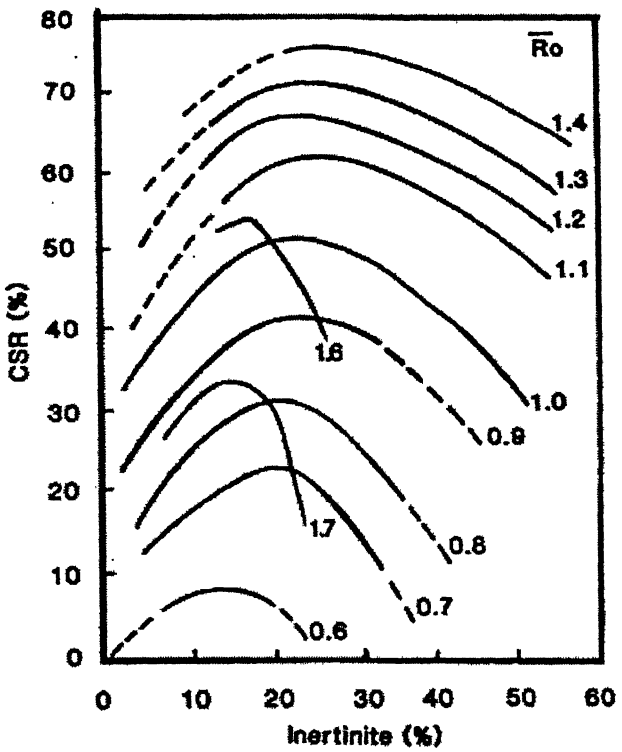


Figure 2.8: NSC CSR Prediction Method

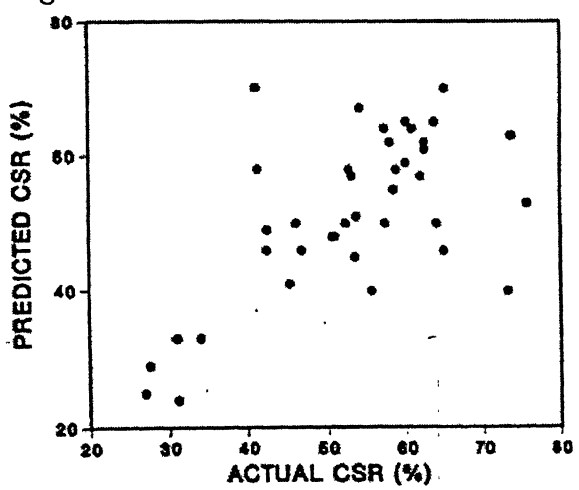


Figure 2.9: NSC Prediction Method Comparison Plot

$$RSI = 70.9 \times Mean\,reflectance\,of\,vitrinite + 7.8 \times \log(max.\,fluidity) - 89 \times \left[\frac{Fe_2O_3 + K_2O + Na_2O + CaO}{SiO_2 + Al_2O_3}\right] - 32 \quad (2.19)$$

$$CSR = RSI - 10 \quad (2.20)$$

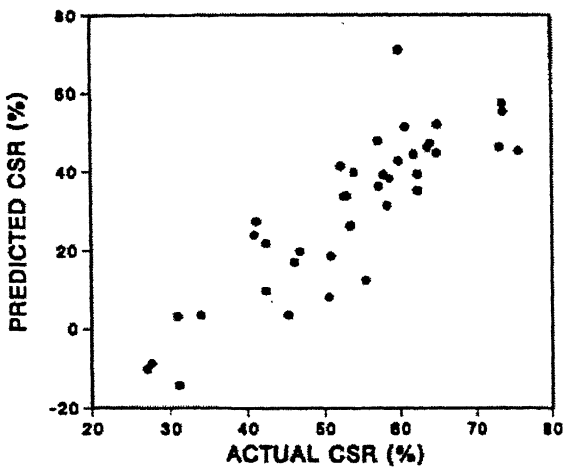


Figure 2.10: Kobe Steel CSR Prediction Method Comparison Plot

The correlation coefficient was 0.74 and standard deviation was 10.75 as shown in Figure 2.10. As reflectance and maximum fluidity are correlated [18], the high covariance produced a higher coefficient of determination. It can be seen [13][14] that inclusion of reflectance, fluidity and alkalies do not correctly represent all of the factors that control CSR.

British Steel [19] and BCRA [20] has developed methods for predicting CSR based on formulae involving coke properties. British Steel method involves determination of coal reflectance and coke ash content while BCRA method involves determination of coal oxygen and carbon content, maximum fluidity, inertinite, alkalies and number of pores per square centimeter in coke.

The NSC and Kobe prediction methods are inadequate as they do not fully account for all of the coal quality parameters that control CSR. The prediction methods developed by BSC, BCRA and NKK take into account coke properties in their prediction formulae, hence CSR cannot be obtained without carborizing the coals.

2.3.3.1.2 Inland Steel CSR Prediction Method A new method developed at Inland Steel [13][14] has been used in this work. According to this method, coal properties can be correlated to two characteristics of coal, namely, plastic range of coal as measured in the Gieseler Plastometer and *Catalytic Index* of CO_2 gasification. Before getting this correlation the effect of a number of coal properties on CSR were studied. The different regression equations obtained are shown in Table 2.6 below.

Table 2.6: Regression Analyses on CSR

S. No.	Regression Equation	R^2	σ
Rheological Parameters			
1.	$CSR = 10.97 + 0.54 \times Plastic\,Range$	0.72	6.6
2.	$CSR = 34.36 + 7.47 \times Maximim\,Fluidity\,(\log DDPM)$	0.58	8.1
3.	$CSR = 32.62 + 34.21 \times FSI\,(\log)$	0.48	9.02
Petrographic Parameters			
4.	$CSR = -90.33 + 225.83 \times Reflectance - 81.70 \times (Reflectance)^2$	0.58	8.2
5.	$CSR = 35.28 + 1.13 \times Organic\,Inerts$	0.22	11.0
Chemical Parameters			
6.	$CSR = 83.58 + 1.27 \times Catalytic\,Index$	0.22	11.04
CSR Prediction Equation			
7.	$CSR = 28.91 + 0.63 \times Plastic\,Range - Catalytic\,Index$	0.80	6.3

Also the graphs showing relationship between the different coal properties and the CSR are shown in Figures 2.11, 2.12, 2.13, 2.14, 2.15, 2.16 and 2.17.

The best model obtained to predict CSR correlates the CSR with *Plastic Range* and *Catalytic Index*. The equation that was developed for CSR prediction is,

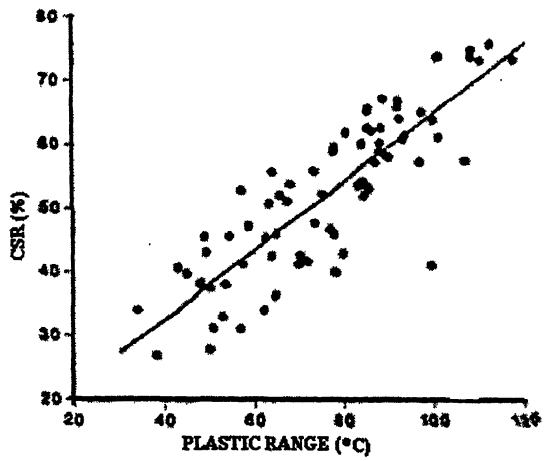


Figure 2.11: Relationship Between CSR and Plastic Range

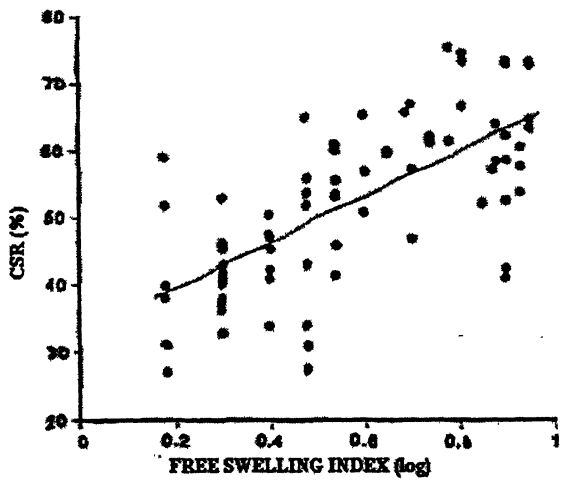


Figure 2.12: Relationship Between CSR and FSI

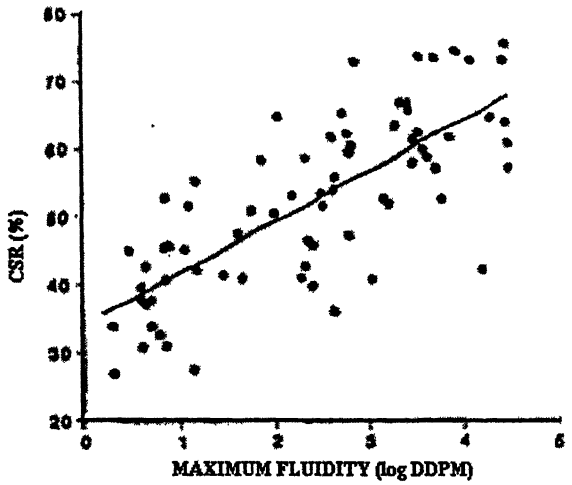


Figure 2.13: Relationship Between CSR and Maximum Fluidity

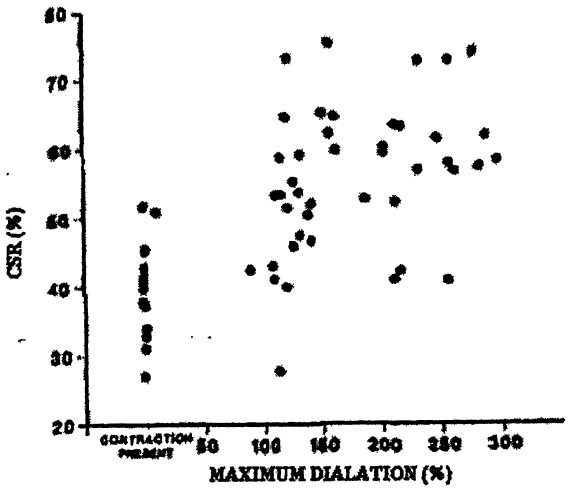


Figure 2.14: Relationship Between CSR and Dilation

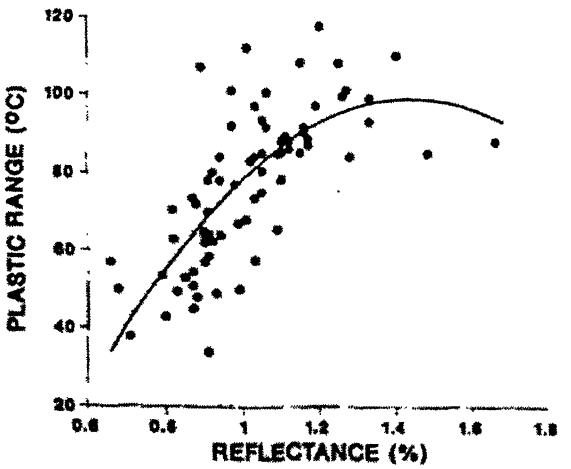


Figure 2.15: Plastic Range versus Reflectance

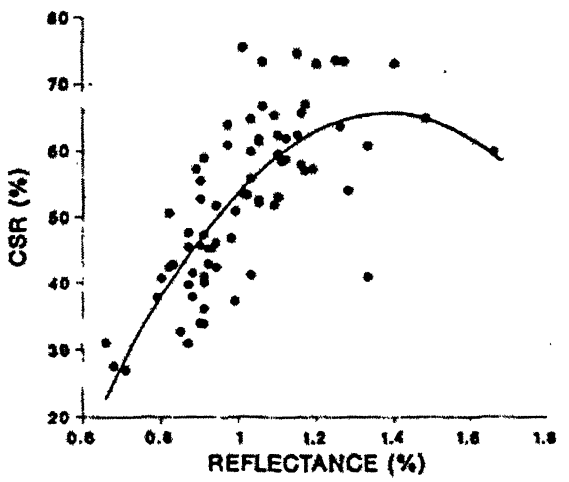


Figure 2.16: Relationship Between CSR and Reflectance

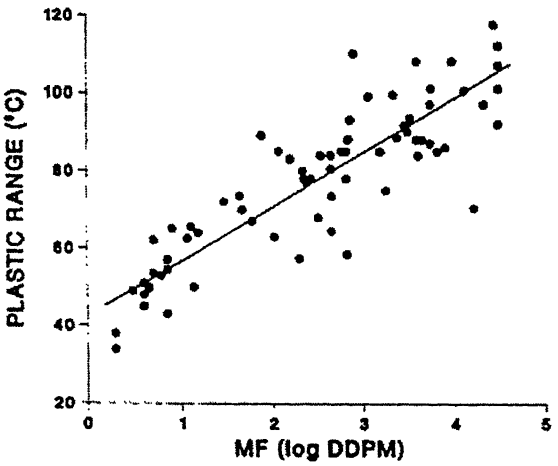


Figure 2.17: Plastic Range versus Maximum Fluidity

$$Coke\ Strength\ after\ Reaction\ (CSR) = 28.91 + 0.63 \times (Plastic\ Range) - Catalytic\ Index \tag{2.21}$$

The *Catalytic Index* comprises of the *Alkali Index* and *Sulfur*, according to the mathematical relationship,

$$Catalytic\ Index\ (CI) = 9.64 \times Alkali\ Index + 14.04 \times Sulfur \tag{2.22}$$

Further, the *Alkali Index* is calculated as,

$$Alkali\ Index\ (AI) = (Ash^{*}\%) \left[\frac{CaO + MgO + Fe_2O_3 + Na_2O + K_2O}{SiO_2 + Al_2O_3}\right] \tag{2.23}$$

$Ash^{*}\%$ is not the ash content calculated from ultimate analysis of coal, but it is the sum of all the oxides present in the coal as calculated using equation 2.24,

$$Ash^{*}\% = SiO_2 + Al_2O_3 + CaO + MgO + Fe_2O_3 + MnO + P_2O_5 + Na_2O + K_2O \quad (2.24)$$

It is seen that CSR increases with an increase in the plastic range and decreases with an increase in the catalytic index. This CSR prediction method works for single coal as well as for blend of coals as CSR is linearly additive [13][14]. Thus, the CSR of coke produced from blended coals can be predicted from individual coal characteristics through the application of additivity law. Calculation procedure followed in Inland for CSR prediction is demonstrated in next section 2.3.3.2.

2.3.3.2 Sample Calculation of CSR for Single Coal

The detailed analysis of the Maple Creek coal is provided below.

Alkali Index is calculated from the chemical composition and plastic range. The plastic range obtained from the Gieseler Plastometer (section 2.1.1) is listed in Table 2.7 below,

Table 2.7: Plastic Properties of Sample Coal Maple Creek

Gieseler Plastometer	
Softening Temperature	$= 382°C$
Solidification Temperature	$= 472°C$
Plastic Range	= Solidification Temperature − Softening Temperature
	$= 472 - 382 = 90°C$

The chemical composition of the coal is also obtained (Tables 2.8 and 2.9). The oxides present in the coal (Table 2.9) are used to calculate the alkali index.

$$Alkali\ Index\ (AI) = (Ash\%)\left[\frac{CaO + MgO + Fe_2O_3 + Na_2O + K_2O}{SiO_2 + Al_2O_3}\right] \quad (2.25)$$

Table 2.8: Chemical Composition of Sample Coal Maple Creek (Ultimate Analysis)

Chemical Composition	
	(%)
$Volatile\,matter$	36.06
Ash	6.610
$Sulfur$	1.280
P	0.011

Table 2.9: Chemical Composition of Sample Coal Maple Creek (Oxides Present)

Chemical Composition	
	(%)
SiO_2	3.454
Al_2O_3	1.744
CaO	0.129
MgO	0.042
Fe_2O_3	0.000
MnO	0.001
P_2O_5	0.024
Na_2O	0.038
K_2O	0.102
Ash^*	5.534

$$= (5.534)\left[\frac{0.129 + 0.042 + 0.000 + 0.038 + 0.102}{3.454 + 1.744}\right]$$

$$= (5.534)\left[\frac{0.311}{5.198}\right]$$

$$AI = 0.331 \tag{2.26}$$

Now, the catalytic index is found out using the AI calculated above in equation 2.26 and $Sulfur$ (from Table2.8),

$$Catalytic\,Index\,(CI) = 9.64 \times (AI) + 14.04 \times (Sulfur) \tag{2.27}$$

$$= 9.64 \times (0.331) + 14.04 \times (1.28)$$

$$CI = 21.163. \tag{2.28}$$

Hence, CSR is predicted using the following relationship,

$$CSR = 28.91 + 0.63 \times (Plastic\,Range) - CI \tag{2.29}$$

$$= 28.91 + 0.63 \times (90) - 21.163$$

$$CSR = 64.447 \tag{2.30}$$

Chapter 3

A Brief Introduction to Genetic Algorithms

3.1 Introduction

Genetic Algorithms were invented to mimic some of the processes observed in natural evolution. The idea with GA is to use this power of evolution i.e. "the survival of the fittest" to solve optimization problems. The father of the original Genetic Algorithm was John Holland who invented it in the early 1970's. Since then the versatality of GA has been proven in almost all disciplines and ample literature [21][22][23] exists on the fundamental as well as applied aspects of GA. Lot of material is available floating on the Internet [24][25][26][27][28][29].

Genetic Algorithms (GAs) are adaptive heuristic search algorithm based on the evolutionary ideas of natural selection and genetics. As such they represent an intelligent exploitation of a random search used to solve optimization problems. Although randomised, GAs are by no means random, instead they exploit historical information to direct the search into the region of better performance within the search space.

The basic techniques of the GAs are designed to simulate processes in natural systems necessary for evolution, and closely follows the principle by Charles Darwin "survival of the fittest". Since in nature, competition among individuals for scanty resources results in the fittest individuals dominating over the weaker ones.

The essential difference between GA and traditional optimization techniques are as follows:

1. Genetic Algorithms (GA) differ from the traditional search and optimization procedures in numerous ways. Basically, most of the traditional procedures are gradient-based, i.e. starting from an initial guess vector, the search algorithm proceeds iteratively toward the optimal point taking the gradient information into account in the N-dimensional search space.

2. Genetic algorithms works by coding of the design variables, which are called individuals. This is very uncommon in traditional methods. This allows genetic algorithms to be applied to discrete or discontinuous function optimization problems. Since no gradient information is used in GAs, they can also be applied to non-differentiable function optimizations, which makes genetic algorithms} much more robust in the sense that they can be applied to a wide variety of problems.

3. Unlike, many traditional optimization methods, genetic algorithms work with a population of points, which more or less ensures the possibilities of obtaining the global optimal solution for any given problem. GA uses the probabilistic transition rule instead of fixed rules. The group of individuals, called population in genetic algorithms terminology, are guided to the global optimum, by powerful genetic reproduction operators, such as Selection, Crossover and Mutation. The randomness in the genetic algorithms operators has an effect of

producing impartial search direction early on, thereby avoiding a hasty wrong decision values; GAs have a directed search later in the simulation.

4. Genetic algorithms are search procedures which are based on the mechanism of natural genetics and natural selection. The basic principle of genetic algorithm is based upon the quasi-Darwinian principle of survival of the fittest, combined with simulated genetic operators abstracted from nature, where an individual attempts to pass its clone to the next generation and it is evaluated in terms of its fitness which is either the function itself or some appropriate transformation of it. For example, in a maximization problem of a function $F(x)$ in between the upper and lower bounds of the decision variable, $x_i^L \leq x_i \leq x_i^U$, the fitness function $f(x)$ is defined same as $F(x)$, while, for a minimization problem the fitness function is changed to $f(x) = 1/(1 + F(x))$.

5. Several other suitable transformation methods as, $f(x) = -F(x)$ are also available depending upon the nature and complexity of the problem. These transformation methods do not alter the location of the global optimum, but convert the minimization problem into a maximization problem.

6. GAs are more robust as they do not break easily even if the inputs changed slightly, or in the presence of reasonable noise. Also, in searching a large state-space, multi-modal state-space, or n-dimensional surface, a Genetic algorithm may offer significant benefits over more typical search of optimization techniques.

In the present work Carroll's Fortran code [30] has been used.

3.2 Algorithm

GA implementation is simple. An initial population is generated randomly, then the algorithm evolves through three operators, namely: Selection – which equates to survival of the fittest, Crossover – which represents mating between individuals, and Mutation – which introduces random modifications. The GA parameters are discussed in detail in Appendix B.

Pseudo-code for Genetic Algorithm

1. randomly initialize population(t)
2. determine fitness of population(t)
3. repeat
   (a) select parents from population(t)
   (b) perform crossover on parents creating population(t+1)
   (c) perform mutation of population(t+1)
   (d) determine fitness of population(t+1)
4. until best individual is good enough

Previously, it has been said that via the operations of selection, crossover, and mutation the GA will converge over successive generations towards the global (or near global) optimum. These simple operations should produce a fast, useful and robust techniques is largely due to the fact that GAs combine direction and chance in the search in an effective and efficient manner. Since population implicitly contains much more information than simply the individual fitness scores, GAs combine the good

information hidden in a solution with good information from another solution to produce new solutions with good information inherited from both parents, inevitably leading towards optimality making GA a powerful, robust optimization technique.

3.3 Micro GA (μGA)

A Simple Genetic Algorithms (SGA) works with a serially implemented binary coded population of size N, with a generation to generation evolution based on selection, crossover and mutation. For the function optimization problems, where the function to be optimized is well defined and do not change faster than the evolution process itself, SGA can be implemented very easily. SGA therefore can handle a stationary function optimization problem quite satisfactorily to find the exact optimum. However, for a non-stationary function optimization problem, where the functions to be optimized are themselves evolving at a much faster rate, SGA can not find an optimum. Problems of this type are found in many real world situations, such as in aerospace (pursuit and evasion), on-line air-craft trajectory optimization, and the optimal control of a aircraft in wind shear etc. Goldberg has proposed that for serial implementation of binary GAs the optimal population choice is small, which was obtained from optimizing effective real-time schema processing in a given population. He also pointed out that simply by taking a small population size and letting them converge is not very useful and outlined a scheme by which a small population GA can be implemented. Based on this approach, a step by step procedure for the μGA implementation, as proposed by Krishnakumar [31] is given below.

1. Select a population of size 5 either randomly or 4 randomly and one good string from any previous search.

2. Evaluate fitness and determine the best string. Label it as string 5 and carry it

to the next generation (elitist selection strategy). In this way there is guarantee that the information about good schema is not lost.

3. Choose the remaining four strings for reproduction (the best string also competes for a copy in the reproduction) based on a deterministic tournament selection strategy [22]. Since the population is small, the law of averages does not hold good and the selection procedure is purely deterministic. In the tournament selection, the strings are grouped randomly and adjacent pairs are made to compete for the final four (care should be taken to avoid two copies of the same string mating for the next generation).

4. Apply crossover with probability of crossover one or near to one. This is done to facilitate a high order of schema processing. The mutation rate is kept to zero as it is clear that enough diversity is introduced after every convergence through new population of strings.

5. Check for nominal convergence. If converged go to first step , else proceed.

6. Go to second step.

7. In implementing μGA, our interest is purely to find the optimum as quickly as possible and not in the average behaviour of the population. The "start and restart" procedure helps in avoiding the premature convergence and μGA is always looking for better strings.

3.4 Sample GA Run

The Carroll's code [30] was used with following GA parameters for optimizing the blends. As an example, the GA parameters for blend having all six coals (combination

15 in Table 5.3) are listed below:

total number of parameters evaluated	6
total binary string length	60
	(10 for each parameter)
population	60
(with 1 child strings kept for the next generation)	
mutation probability	0.00007
crossover probability	0.9
maximum generations	500

Tournament selection, with uniform crossover and elitist selection is used.

The lower and upper bounds set for different coals are listed in Table 3.1.

Table 3.1: Lower and Upper Bounds for Different Coals

Coal	Lower bound	Upper bound
Maple Creek	0.0	70.0
Terry Eagle	0.0	70.0
Wells	0.0	70.0
Amburgy	0.0	70.0
Riverside Sewell	10.0	40.0
Maben	10.0	35.0

As an example, the variation of penalized cost (sum of the total cost of coal blend and penalty terms for all constraint violations) with the number of generations is shown in Figure 3.1 for combination 15 (crossover probability = 0.90; mutation probability = 0.00007).

The blend composition obtained by GA optimization is: Maple Creek (5.47%), Terry Eagle (10.95%), Wells (26.48%), Amburgy (2.88%), Riverside Sewell (29.56%)

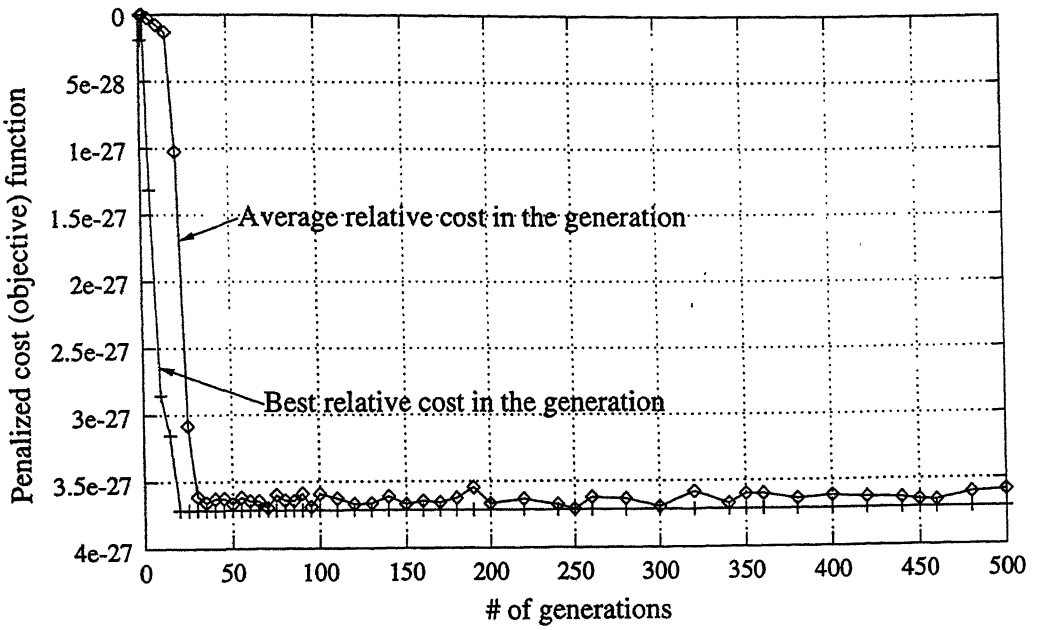


Figure 3.1: Penalized relative cost at different generations for coal combination 15

and Maben (24.66%). Similarly the optimization has been carried out for all the possible coal combinations.

Chapter 4

Problem Formulation

4.1 Problem Description

In an iron and steel plant, the coal is supplied by a number of vendors. The different sources lead to different types of coals. The coals with varying physical, chemical and rheological properties are mixed/blended before their use in the plant. Most coal users follow the practice of coal blending in order to reduce the cost and also to conserve the high quality coals. This is also done because a single coal may not meet with all the requirements of coke quality. The challenge, to the cokemaker is to design a blend which on carbonization would would produce a low-cost-high-quality coke. In the near future more and more rigid coke quality requirements will be faced by cokemakers as iron and steel industry tries to increase productivity and reduce costs by reducing the coke rate.

Coals from six different origins were considered In the present work. The various properties of these coals are listed in Table 4.1.

Table 4.1: Data for Six Coals Used in Optimization

Coals →		Maple Creek	Terry Eagle	Wells	Amburgy	Riverside Sewell	Maben
Coal type based on Volatile Matter (%)		High 36.06	High 34.54	High 34.05	High 37.08	Medium 22.09	Low 16.37
Cost ($)		**31.17**	**39.95**	**37.88**	**36.85**	**45.00**	**43.00**
CSR		64.447	66.816	74.855	55.895	69.788	46.258
Alkali ($Na_2O + K_2O$)		0.140	0.208	0.111	0.149	0.115	0.128
Ash from	Ultimate analysis (%)	6.61	6.71	5.59	5.98	3.96	5.91
	sum of Oxides (%)	5.534	5.386	4.794	5.410	3.813	5.386
Sulfur (%)		1.28	0.67	0.88	0.66	0.73	0.72
Predicted Stability		54.95	59.29	58.37	49.69	59.02	41.87

4.2 Formulation of Optimization Problem

The objective of the optimization problem in the present work was to obtain a blend composition such that the total cost of the blend is minimized subject to certain constraints of quality. The objective function may be represented as shown in equation 4.1.

$$Objective\ function = \min(Total\ Cost\ of\ Blend) \tag{4.1}$$

The cost is to be minimized subject to a number of constraints (see Table 4.2).

The coals are classified into three types based on their mean reflectance and the percent volatile matter present as;

1. High volatile (HV), mean reflectance <1.1; volatile matter 30 - 40%,
2. Medium volatile (MV), mean reflectance 1.1 - 1.3; volatile matter 22 - 30%, and
3. Low volatile (LV), mean reflectance 1.3 - 1.8; volatile matter 14 - 22%.

The requirement for the blend was to have a minimum of 40% and a maximum of 70% of high volatile coal fraction (see constraint equations 4.8 and 4.9 below). The

percentage of medium volatile coals can vary between 10% and 40% of the total blend composition giving two constraint equations 4.10 and 4.11. The limits of low volatile coal fraction are minimum 10% and maximum 35%, which lead to constraint equations 4.12 and 4.13.

In the blend, the properties of coal as CSR, predicted stability, ash content are linearly additive. The coal blend should have an ash content of less than 9.0% (constraint 4.2). The total sulfur should not exceed more than 0.82% (constraint equation 4.3). Minimum CSR of the blend should be 61 (constraint equation 4.4) while predicted stability should be minimum 50 (constraint equation 4.5). Also the alkali in blend (which here includes sum of K_2O and Na_2O fractions fro the chemical analysis) should not exceed 0.40%, leading to another constraint equation 4.6.

Finally, all the fractions should add upto 100%, which is the only equality constraint (equation 4.7) in this problem.

Table 4.2: List of Constraints

$$\begin{aligned}
Ash\,in\,Blend &\leq 9.0 && (4.2)\\
Total\,Sulfur\,in\,Blend &\leq 0.82 && (4.3)\\
CSR\,of\,Blended\,Coal &\geq 61 && (4.4)\\
Coal\,Blend's\,Predicted\,Stability &\geq 50 && (4.5)\\
Alkali\,(K_2O + Na_2O)\,in\,Blend &\leq 0.40 && (4.6)\\
Sum\,fractions\,of\,high,\,medium\,and\,low\,volatile\,coals\,(\%) &= 100.0 && (4.7)\\
Total\,High\,Volatile\,coals\,fraction\,(\%) &\geq 40.0 && (4.8)\\
Total\,High\,Volatile\,coals\,fraction\,(\%) &\leq 70.0 && (4.9)\\
Total\,Medium\,Volatile\,coals\,fraction\,(\%) &\geq 10.0 && (4.10)\\
Total\,Medium\,Volatile\,coals\,fraction\,(\%) &\leq 40.0 && (4.11)\\
Total\,Low\,Volatile\,coals\,fraction\,(\%) &\geq 10.0 && (4.12)\\
Total\,Low\,Volatile\,coals\,fraction\,(\%) &\leq 35.0 && (4.13)
\end{aligned}$$

The penalty function method [23] has been used to incorporate the constraints in

the optimization problem. The constrained optimization problem is thus changed to unconstrained optimization problem by using penalty function method. In a more generalized form, consider a non-linear problem with the objective function $f(x)$ (where, x is an N-dimensional array), subject to inequality constraints $g_j(x)$, $j = 1, 2, , J$, and equality constraints $h_k(x)$, $k = 1, 2, , K$. The problem can be written as,

$$\begin{aligned} &Minimize && f(x) \\ &subject\,to && g_j(x) \geq 0 \quad j = 1, 2, \ldots, J \\ & && h_k(x) = 0 \quad k = 1, 2, \ldots K \end{aligned}$$

A penalty term is added to the objective function,

$$P(x, R^*) = f(x) + \omega(R^*, g(x), h(x))$$

where,

R^* is a set of penalty parameters and

ω is the penalty term chosen. Here a *parabolic penalty* for equality constraints and a *bracket operator penalty* for inequality constraints. Thus,

$$\begin{aligned} Parabolic\,penalty: \quad \omega = \; & R^* \{h(x)\}^2 \\ Bracket\,operator\,penalty: \quad \omega = \; & R^* \langle g(x) \rangle^2 \end{aligned}$$

where, $\langle \alpha \rangle = \alpha$, when α is negative, *zero* otherwise. The value of penalty parameter R^* is fixed by trial and error method.The value of parameter R^* is increased if the

corresponding constraint is not satisfied in the obtained solution. In the present problem a very high value of R^* was needed to satisfy the equality constraint (constraint equation 4.7).

All the inequality constraints are converted to "$\geq$" form and equality constraints are broken into inequality constraints. The constraint in equation 4.7,

$$Sum\ fractions\ of\ coals\ (\%) = 100.0 \tag{4.14}$$

is broken into two inequality constraints as;

$$Sum\ fractions\ of\ coals\ (\%) \geq 99.9 \tag{4.15}$$

$$Sum\ fractions\ of\ coals\ (\%) \leq 100.1 \tag{4.16}$$

In present problem, out of the six coals, four were high volatile coals (Maple Creek, Terry Eagle, Wells and Ambergy) and one each was medium (Riverside Sewell) and low volatile (Maben). In order to satisfy the condition that blend must have atleast one coal of each type the total number of possible combinations have been calculated and found out to be 15 { $(1\times1\times({}^4C_1+{}^4C_2+{}^4C_3+{}^4C_4)) = (1\times1\times(4+6+4+1)) = 15$ }. The optimization was carried out for all the 15 possible combinations and the results are given in chapter 5.

Chapter 5

Coal Blend Optimization: Results and Discussion

5.1 Modeling of Prediction Graphs

The graphs which are used in the prediction of coke stability viz. optimum ratio graph (see Figure 2.4), strength indices graph (see Figure 2.5) and stability graph (see Figure 2.6) are modeled to make the empirical graphs as a part of the computer program which can automatically calculate the stability of the coal under consideration. Various tools (viz. curve-fitting, FAM, etc.) have been used to model the above mentioned three curves, in this work.

5.1.1 Optimum Ratio Graph Model

The curve of optimum ratio graph has been modeled using standard curve fitting routine developed by GNU [32] (available as *Gnuplot* with all releases of Linux Operating System. In the present work Red Hat Linux release 5.1, Gnuplot version 3.5 patchlevel beta 347 was used). This uses the standard Marquardt-Levenberg algorithm

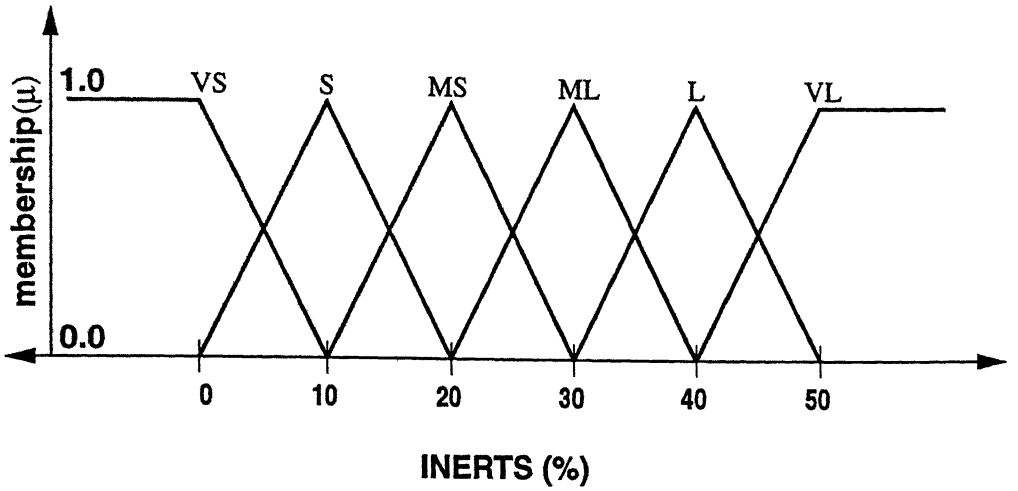


Figure 5.1: Membership function for the Inerts (%) in the Strength Index Chart

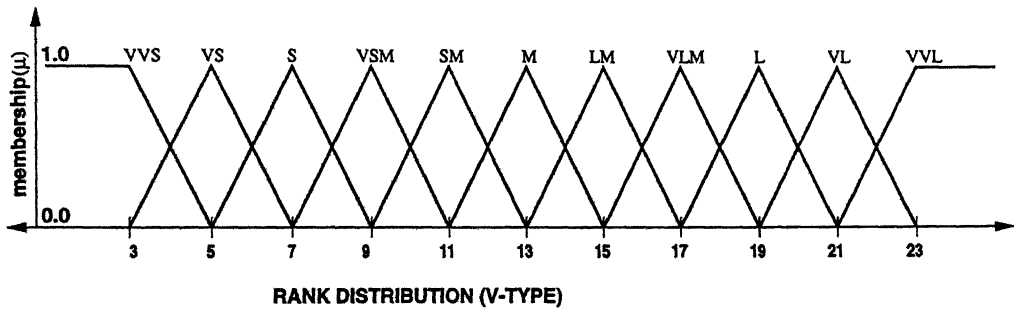


Figure 5.2: Membership function Indices for the Rank Distribution (V-Type) in the Strength Index Chart

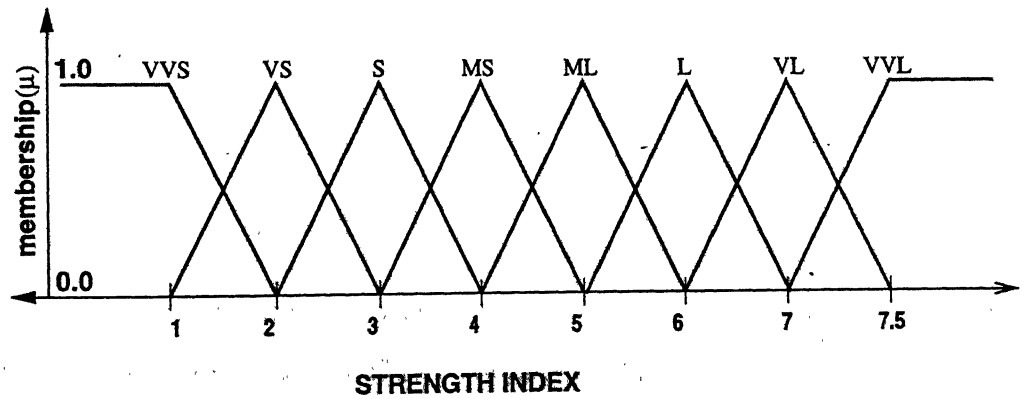


Figure 5.3: Membership function for the Strength Indices in the Strength Index Chart

$$(V\,Type == Large\,(L))\;and\;(Inerts\% == VerySmall\,(VS))$$

then,

$$(Strength\,Index = Large\,(L))$$

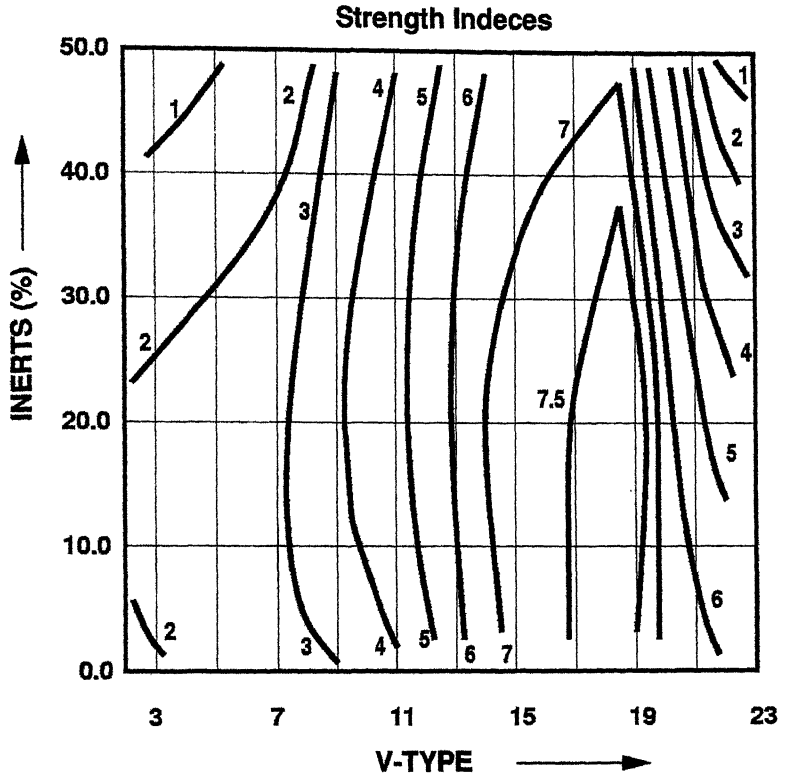
Table 5.1: The FAM Table

Optimum Inerts (%)											
	VL	VVS	VVS	VS	S	MS	ML	L	L	VL	VS	VVS
	L	VVS	VS	VS	S	MS	L	VL	VL	VL	VS	VS
	ML	VS	VS	S	MS	ML	L	VL	VL	VVL	S	S
	MS	VS	S	S	MS	ML	L	VL	VVL	VVL	MS	MS
	S	S	S	S	S	MS	ML	VL	VVL	VVL	ML	ML
	VS	VS	VS	S	S	MS	L	VL	VVL	L	L	L
		VVS	**VS**	**S**	**VSM**	**SM**	**M**	**LM**	**VLM**	**L**	**VL**	**VVL**
		Rank Distribution (V-Type)										

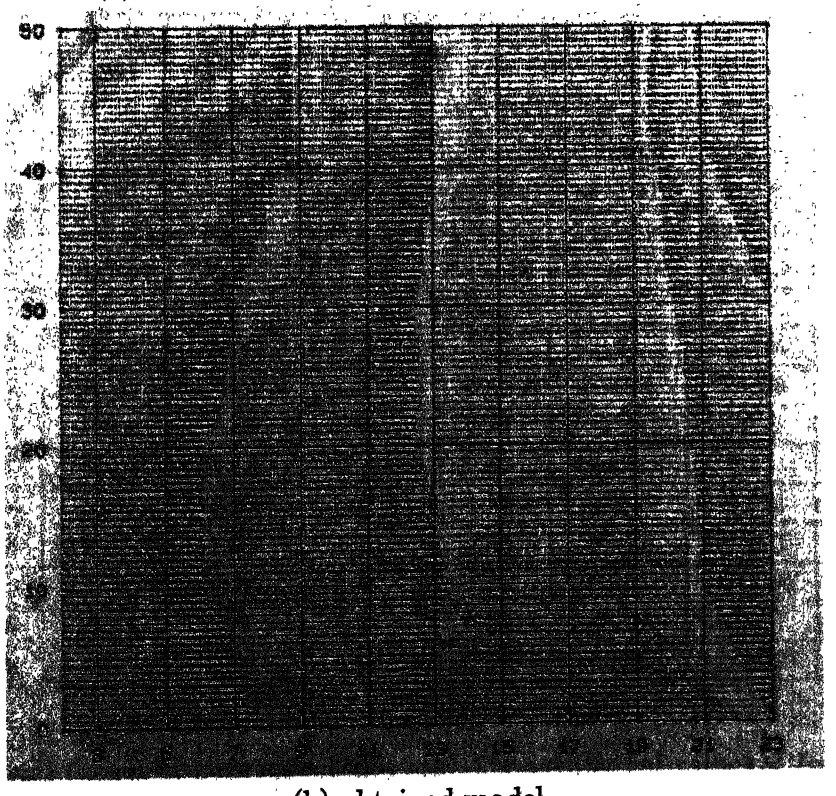
The table 5.1 shows the rule base developed in the present work. The model thus generated is tested by generating a uniform grid of large number of points over the whole x range (Rank distribution (V-type)), y range (Inerts (%)). At each point (x, y) a value of Strength Index is calculated by using the fuzzy model. The output of the model is shown below (see Figure 5.4).

5.1.3 Stability Graph Model

Non-linear least squares method [34] using Marquardt-Levenberg algorithm [33] was used for modeling the curves of the Stability graph. The general form of equation fitted was found to be:



(a) actual graph (refer section 2.3.1, Figure 2.5)



(b) obtained model

Figure 5.4: Model of Strength Indices Chart

$$y = A + B \times x + C \times x^2 + D \times x^3 + E \times x^4 + F \times x^5 + G \times x^6 + H \times x^7 + I \times x^8$$

where, A, B, C, D, E, F, G, H and I are constants separately determined by curve fitting for various curves of the Stability graph (see Figure 2.6).

The summary of the model equations applicable at different stability values obtained by Gnuplot curve fitting is shown in Table 5.2.

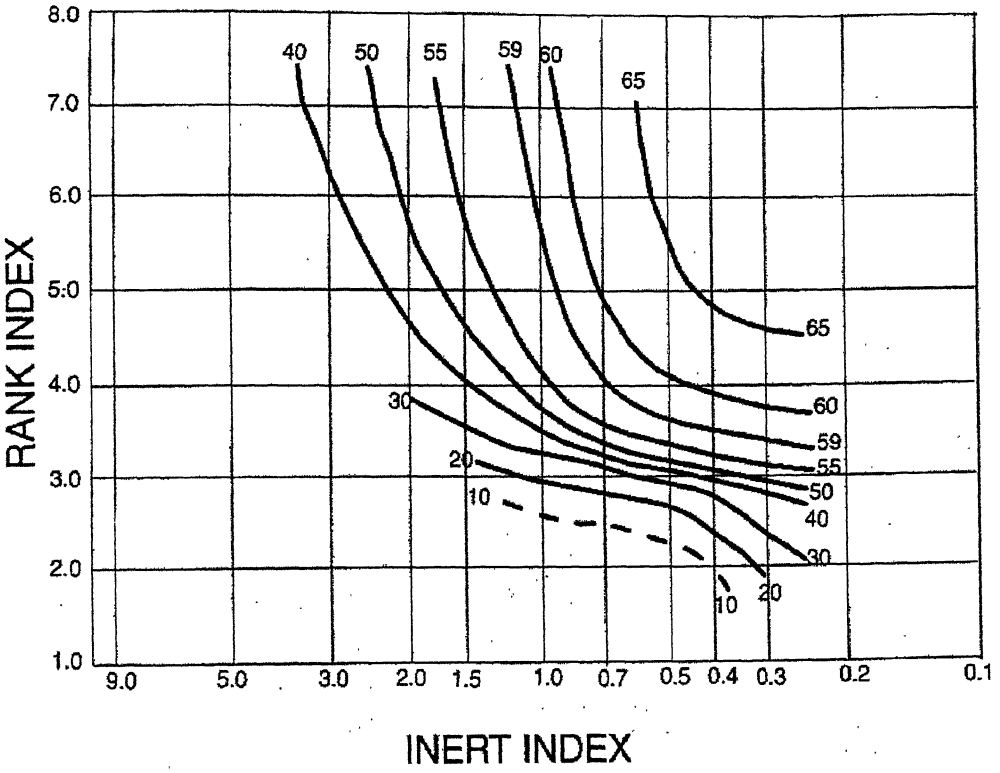
Table 5.2: Stability graph equations

for Inert Index ≤ 1.0									
Stability	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*
65	4.40	-1.49	9.42	138.82	-1173.72	3417.70	-4504.16	2766.25	-645.29
60	3.50	-7.57	147.57	-1009.39	3539.06	-6914.37	7595.56	-4362.23	1015.89
59	2.90	-3.91	82.74	-492.21	1528.80	-2703.31	2721.79	-1441.14	310.03
55	1.54	13.46	-44.76	67.83	-4.84	-127.82	179.09	-101.97	21.63
50	1.16	17.09	-71.70	168.08	-211.79	115.50	23.03	-55.78	18.18
40	1.36	1.27	73.65	-431.95	1148.90	-1692.06	1422.86	-640.11	119.58
30	-3.46	67.46	-398.15	1466.12	-3326.94	4613.71	-3797.87	1701.47	-319.08
20	16.05	-261.27	1747.33	-5978.52	11944.80	-14528.90	10607.00	-4274.09	730.64
10	77.71	-1149.58	7060.07	-23496.10	46982.30	-58214.30	43840.30	-18400.80	3302.94
for Inert Index > 1.0									
65	1.92	16.19	-10.19	5.69	-1.86	0.34	-0.036	0.0020	-0.000046
60	-5.76	21.20	-10.07	2.96	-0.39	0.0014	0.0056	-0.00056	0.000018
59	-1.13	7.99	-0.76	-0.91	0.56	-0.14	0.018	-0.0012	0.000032
55	19.30	-46.64	51.18	-26.05	7.45	-1.25	0.12	-0.0066	0.00015
50	1.23	5.49	-5.80	3.94	-1.30	0.23	-0.023	0.0012	-0.000027
40	1.68	2.97	-1.80	0.79	-0.15	0.012	0.000016	-0.000062	0.0000026
30	2.53	1.34	-1.21	0.84	-0.28	0.053	-0.0056	-0.00030	-0.000007
20	2.69	-0.24	0.79	-0.37	0.10	-0.016	0.0017	-0.000091	0.0000020
10	1.94	0.80	-0.24	0.13	-0.035	0.0045	-0.00024	0.0000005	0.0000003

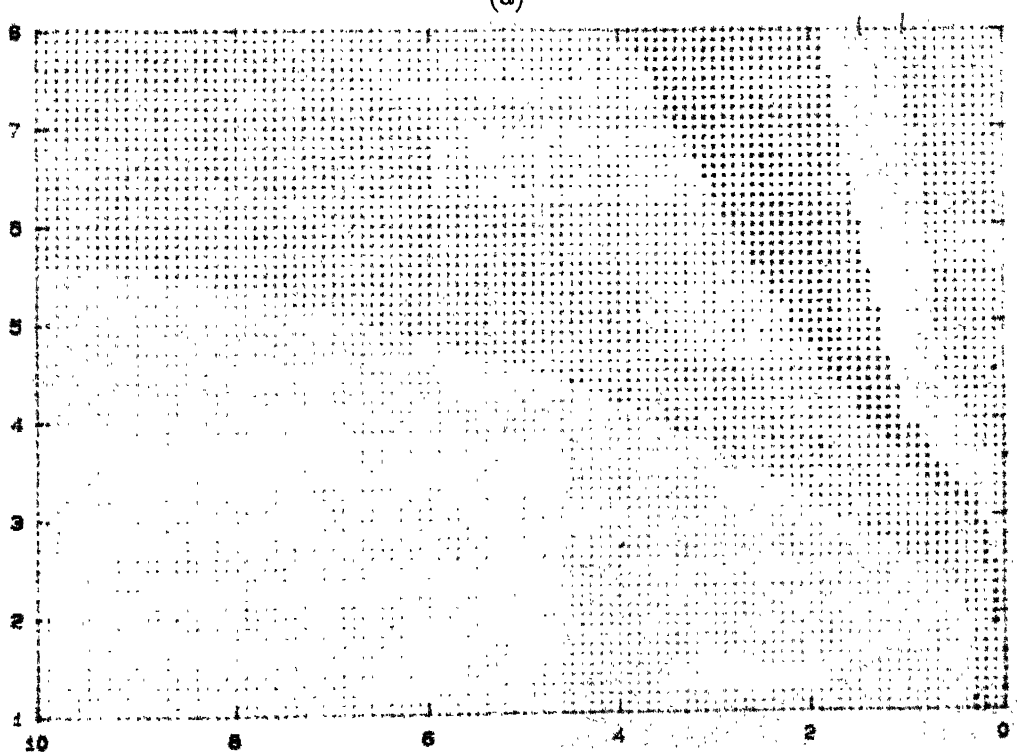
The model was tested by back calculating stability at different values of *Inert Index* and *Rank Index* by generating a uniform grid of points over the entire range of Stability prediction graph (Figure 2.6). The output of the model is shown in Figure

5.5.

The U. S. Steel stability prediction graph (Figure 2.1) was also modeled in the same manner as discussed above. The model obtained ris shown in Figure 5.6 below.

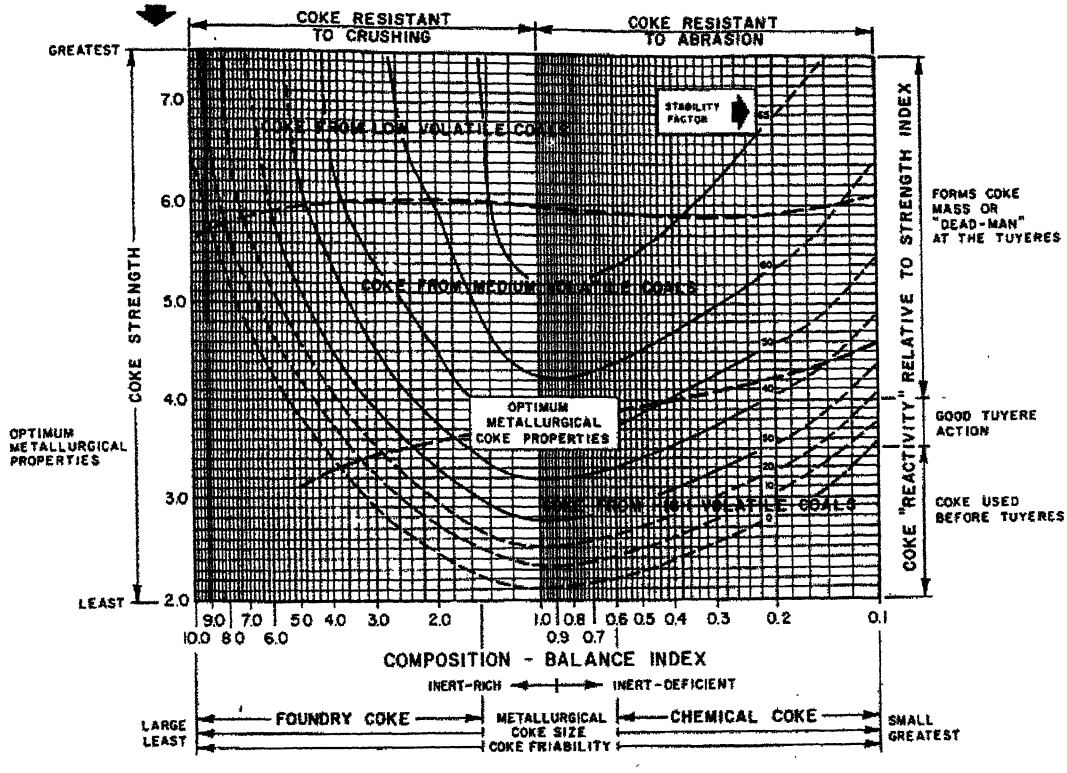


(a)

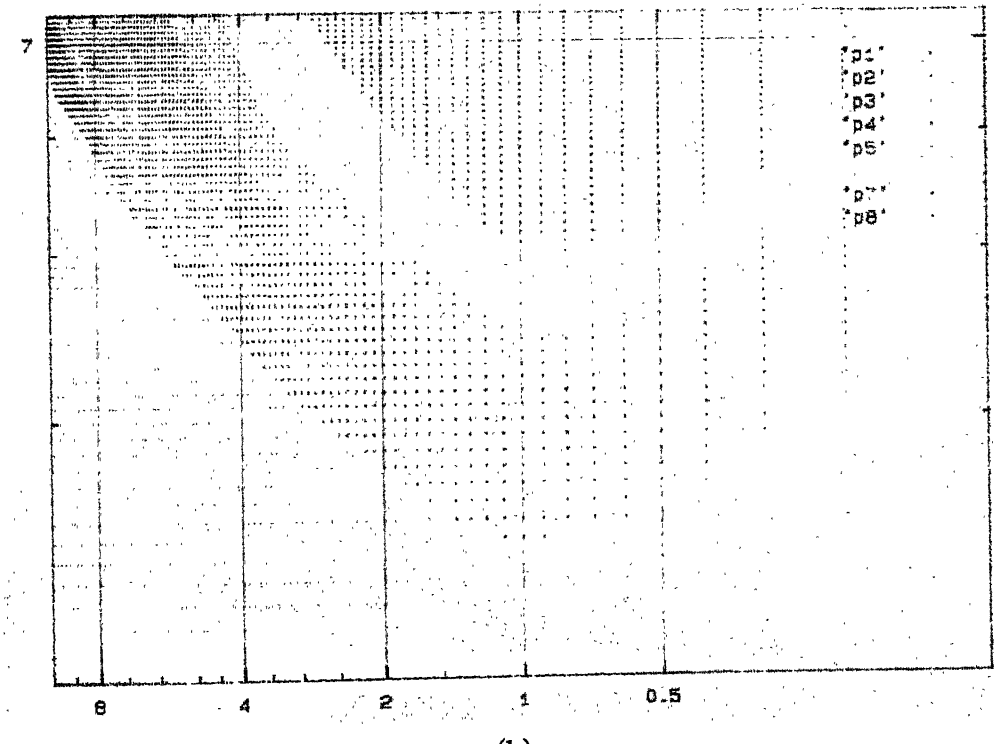


(b)

Figure 5.5: Model of Stability Graph



(a)



(b)

Figure 5.6: Model of U. S. Steel Stability Prediction Graph

5.2 Coal Blend Optimization Results

All the six coals for all the possible 15 blends were optimized using GA. The GA parameters used in different optimization runs are listed in Table 5.3.

Table 5.3: GA Parameters

Coal Combination	Population Size	Bit-String Length	# of Generations	Crossover Probability	Mutation Probability
1	50	30	500	0.90	0.0007
2	50	30	500	0.80	0.0001
3	50	30	500	0.80	0.0001
4	35	30	500	0.91	0.00004
5	60	40	700	0.93	0.00002
6	60	40	1800	0.80	0.0002
7	70	40	500	0.94	0.00007
8	40	40	500	0.88	0.00003
9	40	40	500	0.94	0.00002
10	40	40	500	0.90	0.00001
11	50	50	500	0.80	0.00007
12	50	50	500	0.90	0.0002
13	50	50	500	0.94	0.00001
14	50	50	500	0.90	0.00002
15	60	60	500	0.90	0.00007

The results obtained after optimization are as follows (Table 5.4):

All the blends which were obtained after optimizing with GA, they were analysed and results are listed in Table 5.5. The table shows the fractions of each coal present in that particular blend and the analysis of the blend. It is observed that the fractions obtained satisfy almost all the constraints barring a few exceptions like: For Blend Nos. 1, 5, 6, 11, 12, 13 the sulfur constraint is violated; For Blend No. 4 CSR was not satisfied. For the rest of the blends all the constraints were satisfied.

Cost for blend of coals Maple Creek, Riverside Sewell and Maben (Blend No. 1) has the minimum cost of $37.04. The maximum cost of $42.42 was exhibited by

Table 5.4: Optimization Blend Composition Results for Different Possible Coal Combinations

Blend No. ↓	Combinations of Coals	Blend Composition					
		MC[a]	TE[b]	WE[c]	AM[d]	RS[e]	MA[f]
1	MC RS MA	55.25	—	—	—	29.00	15.74
2	TE RS MA	—	42.39	—	—	37.57	19.95
3	WE RS MA	—	—	40.79	—	37.36	21.85
4	AM RS MA	—	—	—	66.69	22.58	10.73
5	MC TE RS MA	40.78	11.84	—	—	30.67	16.70
6	MC WE RS MA	35.03	—	13.14	—	20.65	31.18
7	MC AM RS MA	17.70	—	—	39.59	31.41	11.29
8	TE WE RS MA	—	44.13	26.96	—	11.85	17.06
9	TE AM RS MA	—	36.47	—	7.11	39.53	16.89
10	WE AM RS MA	—	—	45.16	9.44	26.80	18.60
11	MC TE WE RS MA	35.31	9.58	18.95	—	12.84	23.32
12	MC TE AM RS MA	37.29	27.44	—	6.36	15.06	13.84
13	MC WE AM RS MA	35.10	—	10.88	19.16	24.75	10.10
14	TE WE AM RS MA	—	35.65	26.82	5.61	19.88	12.03
15	MC TE WE AM RS MA	5.47	10.95	26.48	2.88	29.56	24.66

[a]MC:Maple Creek [b]TE:Terry Eagle [c]WE:Wells [d]AM:Amburgy [e]RS:Riverside Sewell [f]MA:Mah

blend of coals Terry Eagle, Riverside Sewell and Maben (Blend No. 2).

Considering the blend of all the six coals consisting of Maple Creek, Terry Eagle, Wells, Amburgy, Riverside Sewell and Maben (Blend No. 15) all the constraints are satisfied. But the coals Amburgy and Maple Creek contribute in very small amounts to the final blend. Amburgy is mere 2.88% while Maple Creek is 5.47%. In practice it is not possible to add such a small fractions into the blend. Hence they can be left out. If we remove Amburgy from the blend we get Blend No. 11, which has been optimized with all coals except Amburgy present in the blend. The corresponding effect of removal of Amburgy from the blend could be seen by comparing the blend analysis. The cost of Blend No. 11 is less $37.82 as compared to $41.08 of Blend No. 15. The effect of removal of Amburgy is that sulfur constraint gets violated. Also the ash content of the coal increases slightly from 4.77 to 5.12 while the CSR decreases from 64.31 to 63.09. Coal Amburgy is a low sulfur (0.66) coal, with low CSR (55.895). Hence it's removal increased the sulfur amount in the blend and sulfur limit got violated. The characteristics of each coal is listed in Table 4.1, which is reproduced below.

Data for Six Coals Used in Optimization							
Coals →		Maple Creek	Terry Eagle	Wells	Amburgy	Riverside Sewell	Maben
Coal type based on Volatile Matter (%)		High 36.06	High 34.54	High 34.05	High 37.08	Medium 22.09	Low 16.37
Cost ($)		**31.17**	**39.95**	**37.88**	**36.85**	**45.00**	**43.00**
CSR		64.447	66.816	74.855	55.895	69.788	46.258
Alkali ($Na_2O + K_2O$)		0.140	0.208	0.111	0.149	0.115	0.128
Ash from	Ultimate analysis (%)	6.61	6.71	5.59	5.98	3.96	5.91
	sum of Oxides (%)	5.534	5.386	4.794	5.410	3.813	5.386
Sulfur (%)		1.28	0.67	0.88	0.66	0.73	0.72
Predicted Stability		54.95	59.29	58.37	49.69	59.02	41.87

If we look at Blend No. 14 in which Maple Creek has been left out (contribution

of Maple Creek is only 5.47% in Blend No. 15) there is not much significant change in the blend characteristics except that CSR has improved slightly from 64.31 to 66.47 and cost has gone down from $ 41.08 to $ 40.59. Also it is observed that in Blend No. 14 coal Amburgy contributes in very small amount (5.61%).

Thus, removing both Maple Creek and Amburgy form the blend of coals, we get a blend of remaining four coals (Blend No. 8). The blend analysis shows that the cost is average $ 40.51 and the corresponding CSR and stability values are high. CSR is 65.83 (66.71 being the highest) and stability is 56.04 (maximum possible stability obtained for any blend being 56.35). Thus, we have arrived at a suitable blend.

Blend No. 12 is a mix of five coals; Maple Creek, Terry Eagle, Amburgy, Riverside Sewell and Maben. In this blend the amount of Amburgy is 6.36%. If coal Amburgy is left out we get Blend No. 5, which shows an increased cost of $ 38.42 over $ 37.63 of coal Blend No. 12. The CSR and stability show marginal improvement, while ash content has reduced. The coal Amburgy is contributing in small amounts in the blend is because it has low stability (49.69) and CSR (55.895), thus during optimization, to obtain a blend with CSR "> 61" and stability "> 50", contribution of this coal is reduced.

Comparing the Blend Nos. 9 and 2. Blend No. 2 is the blend with highest cost $ 42.42. When coal Amburgy gets added to this blend, though in a small amount of 7.11%, cost gets reduced to $ 42.24. While all the other blend characteristic parameters remain same.

Coal selection is a difficult exercise to do by looking at a table (as Table 5.5). But it becomes lot easier if we use some interactive program, like Java Applet [37]. A coal selector which implements Java Applet was used to carry out coal blend selection. The snapshots of coal selector applet are given in Appendix C.

Blend No. ↓	Blend Composition					Blend Analysis						Cost	Remarks
Goals →	*Maple Creek*	*Terry Eagle*	*Wells*	*Amburgy*	*Riverside Sewell*	*Maben*	Sum	Ash < 9	CSR > 61	Stab > 50	Sul < 0.82	Alk < 0.4	$	
1	55.25	——	——	——	29.00	15.74	99.99	5.01	63.13	54.07	1.03	0.13	**37.04**	Sulfur violated
2	——	42.38	——	——	37.57	19.95	99.90	4.79	63.76	55.65	0.70	0.16	**42.42**	ACS†
3	——	——	40.79	——	37.36	21.85	100.0	4.56	66.71	55.01	0.79	0.12	**41.66**	ACS†
4	——	——	——	66.69	22.58	10.73	100.0	5.05	58.00	50.96	0.68	0.14	**39.35**	CSR violated
5	40.78	11.84	——	——	30.67	16.70	99.99	4.96	63.32	54.52	0.94	0.14	**38.42**	Sulfur violated
6	35.03	——	13.14	——	20.65	31.18	100.0	5.04	61.25	52.16	0.94	0.13	**38.60**	Sulfur violated
7	17.70	——	——	39.59	31.41	11.29	99.99	4.93	60.68	52.66	0.80	0.13	**39.10**	ACS†
8	——	44.13	26.96	——	11.85	17.06	100.0	5.04	65.83	56.04	0.74	0.16	**40.51**	ACS†
9	——	36.47	——	7.11	39.53	16.89	100.0	4.77	63.75	55.56	0.70	0.15	**42.24**	ACS†
10	——	——	45.16	9.44	26.80	18.60	100.0	4.70	66.39	54.66	0.79	0.12	**40.64**	ACS†
11	35.31	9.58	18.95	——	12.84	23.32	100.0	5.12	63.09	53.49	0.94	0.14	**37.82**	Sulfur violated
12	37.29	27.44	——	6.36	15.06	13.84	99.99	5.22	62.55	54.40	0.91	0.15	**37.63**	Sulfur violated
13	35.10	——	10.88	19.16	24.75	10.10	99.99	4.99	63.42	54.00	0.92	0.13	**37.60**	Sulfur violated
14	——	35.65	26.82	5.61	19.88	12.03	99.99	4.92	66.47	56.35	0.74	0.15	**40.59**	ACS†
15	5.47	10.95	26.48	2.88	29.56	24.66	100.0	4.77	64.31	54.16	0.79	0.13	**41.08**	ACS†

†: All Constraints Satisfied

Part II

Coke Rate Prediction

Chapter 6

Coke Rate prediction Models and Plant Data

"Coke rate" or "coke consumption rate" is defined as the amount of coke consumed for producing a unit of blast furnace hot metal in $(kg \text{ or } Tons)/Metric Ton of Hot Metal$. The amount of coke consumed in a day is usually termed as the coke throughput or coke burning rate or driving rate. The coke rate and driving rate are related to the production rate of hot metal,

$$PI = \frac{Q}{K} \tag{6.1}$$

where,

PI is the productivity or hot metal production rate $(Metric Ton of Hot Metal\ (MTHM))$,

Q is the driving rate or coke burned, $(Metric Ton\ (MT)/day)$, and,

K is the coke rate $(kg/MTHM)$.

According to relation 6.1, to increase productivity, coke rate should be less [38] and driving rate should be more [39]. The coke rate effect on productivity and methods to reduce the coke rate have been studied extensively. For example, an increase in blast

temperature is accompanied by a reduction in the coke rate [40]. Also researchers at Urals Research Institute for Ferrous Metallurgy [41] found that introduction of oil into blast furnace through the tuyers with increase in blast furnace temperature and decrease in blast humidity enables coke rate to get reduced and blast productivity to increase. Injection of natural gas into blast furnace [42] also lowers the coke rate. Researchers at Siberian Metallurgical Institute, Russia [43][44] found that coke oven gas injection increases blast furnace production vis-á-vis decrease the coke rate. A reduction in coke rate corresponds to that calculated from B. I. Kitaev equation (see Equation 6.2) multiplied by the coefficients of the relative amount of carbon burnt at the tuyers, C_t.

$$E = \frac{(T_0' - 850) - (T_0' - 850)}{(T_0' - 850)} \times 100 \tag{6.2}$$

where,

E is the measure of coke economy (%),

T_0 is the theoretical flame temperature in front of tuyers before increasing the blast temperature ($^\circ C$), and,

T_0' is the theoretical flame temperature in front of tuyers after increasing the blast temperature ($^\circ C$).

Based on the analysis of blast furnaces around the world an empirical coke rate equation (equation 6.3) has been derived [45].

Empirical coke rate equation is

$$K = C_1 + C_2B + C_3S_r - C_4S - C_5P^* - C_6T \tag{6.3}$$

where,

K is the coke rate ($kg/Metric Ton of Hot Metal\,(MTHM)$),

B is the net burden rate $kg/MTHM$),

S_r is the sinter percentage of gross burden,

$P^{\star}$ is the pellet percentage of gross burden weight (which is 0, since pellets are not charged since pellets are not charged in the plants from which data is taken), and,

T is the blast temperature (K),

In this equation, the C_1, C_2, C_3, C_4, C_5 and C_6 values are the constants for a given blast furnace and are determined by regression analysis from operational data.

Another parameter directly affecting the coke rate is the blast kinetic energy,

$$E_b \propto \frac{V^3 T^2}{P^2}$$

where,

E_b is the kinetic energy of the blast,

V is the blast volume ($Nm^3/second$),

T is the blast temperature (K), and

P is the absolute blast pressure ($atm.$).

In the present work, based on the literature study, the important variables affecting the coke rate were identified as hot blast temperature ($^{\circ}C$), Cold blast flow (Nm^3), blast pressure ($atm.$), slag rate ($kg/MTHM$), top pressure ($atm.$), hot metal production (MT), sinter rate ($kg/MTHM$), iron ore rate ($kg/MTHM$) and lime stone consumption (MT) Coke rate prediction based on these parameters has been carried out.

6.1 Plant Data

The data used for coke rate prediction modeling is daily operational data for Blast furnace No. 1 at Visakhapatnam Steel Plant, Visakhapatnam, India for a period of six months. The operational parameters: Hot blast temperature ($°C$), Cold blast flow (Nm^3), Blast pressure ($atm.$), Slag rate ($kg/MTHM$), Top pressure ($atm.$), Hot metal production (MT), Sinter rate ($kg/MTHM$), Iron ore rate ($kg/MTHM$) and Lime stone consumption (MT), are the independent variables and Coke rate ($kg/MTHM$) is the dependent variable. A set of 182 data is listed in Table 6.1 below. These data are used to predict coke rate by developing various models discussed in chapter 7.

Table 6.1: Data for Coke Rate

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1050	4250	3.00	319	1.70	4001	1168	379	9	530
1050	4250	3.09	354	1.64	2762	1321	419	0	595
1050	3850	2.65	299	1.39	3900	1104	350	0	501
1050	3700	2.59	302	1.39	3393	1124	356	0	505
1050	3750	2.50	301	1.20	3800	1111	352	0	500
1050	3900	2.70	313	1.39	3721	1168	385	0	525
1050	3900	2.84	319	1.64	3660	1147	397	0	525
1050	4200	3.00	310	1.70	3936	1156	390	0	519
1050	4300	3.00	368	1.75	3501	1370	468	0	599
1050	4100	2.95	303	1.70	3490	1155	394	0	513
1050	4200	2.90	306	1.60	3806	1142	399	0	513

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1050	4400	3.90	309	1.70	4559	1167	359	3	517
1050	4300	3.00	302	1.70	3965	1155	330	0	506
1050	4400	3.20	320	1.79	4189	1228	349	5	536
1050	4400	3.20	330	1.79	4037	1270	362	15	550
1050	4450	3.09	311	1.79	4209	1222	316	8	520
1050	4500	3.20	303	1.85	4609	1200	331	7	508
1050	4800	3.20	300	1.85	4589	1185	327	7	501
1050	4800	3.20	331	1.85	4120	1294	361	5	555
1050	4600	3.20	306	1.79	4602	1177	327	0	513
1050	4500	3.20	299	1.79	4300	1155	342	0	501
1050	4900	3.29	328	1.85	4433	1256	387	0	549
1050	4900	3.29	329	1.85	4508	1272	382	0	552
1050	4800	3.29	314	1.85	4736	1179	365	0	527
1050	4800	3.20	288	1.89	4882	1101	341	0	483
1050	4800	3.20	344	1.79	4220	1314	407	0	576
1052	4400	3.20	320	1.79	3366	1210	370	2	554
1045	4400	3.20	298	1.79	4459	1165	325	7	500
1045	4750	3.09	318	1.79	4503	1242	346	8	532
1030	4700	3.09	305	1.79	4579	1193	333	0	509
1040	4600	3.09	316	1.79	4209	1236	345	0	529
1030	4500	3.20	329	1.75	4081	1298	359	0	547
1015	4600	3.20	356	1.79	3672	1398	358	9	593
1005	4650	3.20	294	1.79	4604	1162	321	14	491

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1025	4400	3.09	309	1.75	2779	1203	318	8	526
1035	4600	3.09	288	1.75	4394	1127	314	0	482
1040	4200	2.95	323	1.64	3848	1274	356	0	542
1040	4400	3.09	318	1.70	4116	1243	347	0	534
1030	4250	3.09	317	1.75	3954	1240	346	0	532
1030	4550	3.09	318	1.70	4183	1244	357	0	533
1030	4600	3.20	304	1.75	4600	1199	345	0	509
1040	4700	3.29	301	1.85	4536	1166	339	5	500
1040	4400	3.25	320	1.85	2476	1233	399	0	547
1030	4650	3.20	313	1.79	4108	1230	356	0	525
1035	4200	2.70	342	1.50	3574	1335	381	0	583
1045	4250	2.75	311	1.64	3753	1192	330	0	530
1025	4600	3.29	341	1.85	3871	1333	387	0	572
1038	4500	3.04	313	1.75	4005	1207	334	0	523
1045	4400	3.00	282	1.70	3353	1129	282	0	478
1048	4400	3.09	386	1.70	3249	1554	386	0	646
1030	4500	3.09	308	1.79	4001	1225	305	0	479
1030	4300	3.04	295	1.75	3883	1184	395	0	494
1014	4277	2.93	327	1.64	4110	1304	343	0	547
1011	3950	2.59	324	1.38	3801	1274	320	3	533
1023	4471	2.70	309	1.50	4200	1274	286	0	522
1026	4708	2.71	321	1.60	4040	1344	292	0	538
1040	4712	3.05	313	1.79	4605	1308	268	0	528

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1030	4104	2.24	305	1.32	3539	1315	252	0	507
1032	4061	2.07	333	1.32	2936	1377	264	0	534
1039	4471	2.94	289	1.62	4681	1225	235	0	488
1045	3987	2.67	292	1.42	4328	1227	228	0	498
1049	4578	3.20	339	1.74	4094	1410	253	0	559
1038	4476	2.79	316	1.59	4393	1313	258	0	533
1039	4515	2.96	316	1.69	4385	1299	242	0	537
1038	4216	2.70	317	1.39	4194	1321	244	0	527
1043	4126	2.39	321	1.58	4109	1343	263	0	538
1040	4520	2.56	332	1.70	3942	1377	269	0	550
1038	4499	3.22	320	1.74	4300	1343	268	0	547
1045	4495	2.86	316	1.58	4070	1334	261	0	534
1024	3542	2.70	285	1.42	3632	1178	230	0	494
1029	4615	3.09	317	1.72	4237	1325	259	0	533
1039	4415	2.93	328	1.57	4053	1387	214	1	544
1027	4192	2.77	326	1.47	3776	1424	212	0	547
1050	4717	3.01	345	1.64	4213	1481	226	2	572
1032	4829	2.91	318	1.77	4007	1404	203	8	533
1030	4394	3.05	284	1.78	4304	1251	181	2	479
1050	4701	3.09	317	1.74	4504	1389	200	5	528
1054	4839	3.13	276	1.77	5258	1227	177	8	466
1057	4747	3.00	326	1.67	4216	1485	224	6	572
1050	4574	2.95	284	1.57	4606	1284	190	12	510

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1034	4600	3.09	329	1.70	1670	1557	242	14	595
1045	4700	3.29	333	1.85	2903	1471	213	13	572
1053	4398	2.77	316	1.39	4280	1394	201	7	534
1050	4531	3.09	317	1.68	4331	1389	197	8	528
1050	4299	2.82	314	1.52	4209	1371	191	1	530
1050	3896	2.43	322	1.37	3416	1405	178	8	534
1046	4351	2.86	312	1.53	4193	1382	193	11	527
1033	4610	2.97	334	1.55	4017	1478	213	1	566
1033	4509	2.84	284	1.54	4216	1292	181	0	494
1036	4576	2.89	304	1.65	4159	1383	205	0	523
1032	4512	3.02	293	1.66	4543	1352	190	9	511
1039	4454	2.78	300	1.67	4108	1390	188	13	516
1037	4503	3.01	336	1.63	4060	1558	214	7	577
1035	4586	2.97	319	1.62	4036	1502	214	4	559
1020	3878	2.85	277	1.51	4047	1286	170	12	477
1025	4357	3.11	289	1.72	4116	1312	157	23	483
1028	4503	2.76	295	1.61	4214	1341	161	20	496
1010	4217	2.63	326	1.52	3514	1480	178	15	545
1020	4325	2.93	319	1.56	4033	1451	174	14	535
1006	4146	2.48	284	1.70	3173	945	159	13	488
1005	3641	2.30	298	1.34	3175	1354	163	13	500
986	4175	2.20	378	1.64	2446	2014	197	9	617
1025	3883	2.81	293	1.47	4048	1251	189	0	496

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1032	3799	2.63	321	1.21	3463	1286	282	0	543
1046	4046	2.65	314	1.53	3644	1220	315	5	520
1049	3974	3.14	303	1.68	4109	1183	327	3	506
1047	3057	2.63	339	1.44	2918	1282	358	2	548
1048	3396	1.81	334	1.55	2008	1285	359	0	520
1154	3697	2.80	309	1.51	3815	1279	278	0	526
1019	3934	2.69	306	1.60	3552	1386	271	0	554
1028	3272	2.68	302	1.40	3646	1262	247	0	506
1029	3544	2.67	333	1.40	3538	1391	272	0	557
1033	3173	2.69	304	1.46	3801	1292	239	0	519
1004	3850	2.63	332	1.38	3151	1370	239	0	561
999	2807	2.81	316	1.57	3165	1384	336	0	594
1011	2522	2.77	308	1.52	3574	1219	326	0	515
1018	2358	2.89	315	1.65	3840	1289	286	0	527
1014	3700	2.65	330	1.40	2796	1304	290	0	553
1016	2648	2.64	353	1.43	2772	1392	393	0	611
1023	5033	2.79	325	1.59	3690	1268	384	0	547
1037	6038	3.98	330	1.47	3937	1250	390	2	557
1040	4184	3.09	311	1.79	4001	1186	367	8	521
1043	3700	3.00	370	1.62	2795	1413	421	0	620
986	3723	3.00	319	1.58	3410	1223	324	0	536
960	4000	2.96	325	1.77	3553	1271	295	1	548
956	3700	2.90	324	1.61	3154	1268	280	10	562

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1019	2968	1.81	337	1.40	2250	1300	280	0	589
956	3701	3.00	357	1.59	3018	1412	260	0	620
981	3670	3.00	367	1.73	2671	1338	228	0	562
984	4119	3.09	380	1.78	3553	1330	228	0	568
982	3904	3.04	399	1.78	3586	1279	279	10	545
993	3237	2.60	377	1.69	2802	1228	271	4	542
999	3666	2.39	396	1.69	2722	1256	279	0	562
995	4018	2.07	388	1.72	2408	1338	309	0	597
995	3598	2.52	353	1.43	3143	1272	299	0	549
1001	3350	2.58	327	1.65	3160	1193	294	0	533
999	3361	2.63	382	1.70	2594	1359	365	0	623
1003	3450	2.90	295	1.63	3314	1047	260	0	481
1056	3741	3.00	303	1.67	2840	1167	279	0	556
1003	3795	2.92	333	1.68	3029	1300	333	0	599
1011	3930	3.00	322	1.75	3419	1245	319	0	557
1005	4250	2.99	334	1.73	3681	1251	318	0	570
1005	4158	3.00	325	1.74	4002	1229	322	0	551
1017	4246	3.00	304	1.69	3904	1158	304	0	519
1005	4284	3.09	310	1.82	4001	1200	310	0	529
1009	4205	3.00	330	1.67	3750	1290	331	0	564
1007	4000	3.00	318	1.79	3739	1173	289	0	513
1013	4100	2.98	363	1.76	3666	1376	336	0	602
1012	4227	3.09	294	1.80	4184	1127	275	0	492

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1015	4502	3.10	339	1.86	4186	1263	308	0	552
1015	4446	3.05	334	1.78	3963	1307	315	0	571
1017	4246	3.10	314	1.87	4309	1185	285	0	511
1018	4174	3.07	358	1.83	3744	1352	326	0	583
1016	3501	2.39	348	1.60	2592	1321	328	0	576
1032	3963	2.92	341	1.73	3576	1269	357	0	556
1022	3932	2.96	329	1.77	3782	1255	299	0	543
1012	4146	3.20	340	1.88	3559	1298	309	0	554
1014	4289	3.07	314	1.86	4375	1200	286	0	512
1021	4388	3.15	343	1.87	4107	1309	312	0	559
1021	4305	3.13	319	1.88	3888	1404	319	0	550
1023	4263	3.20	307	1.87	3945	1339	307	0	550
1029	4334	3.11	302	1.88	4590	1195	277	6	504
1024	4365	3.17	352	1.95	3840	1409	320	8	590
1013	4000	3.15	290	1.76	3206	1276	284	0	540
1021	4239	3.03	315	1.82	4012	1228	287	0	514
1031	4345	2.97	317	1.73	4169	1266	288	0	530
1018	4292	3.04	312	1.82	4264	1238	281	0	523
1024	4192	3.06	291	1.81	4383	1175	267	0	492
1029	4047	3.00	303	1.80	3630	1321	300	0	559
1030	4476	3.09	293	1.83	4270	1260	321	0	539
1027	4173	3.03	291	1.78	4093	1261	323	0	540
999	4280	3.60	321	1.87	4110	1266	324	0	543

Hot Blast Temp.	Cold Blast Flow	Blast Pres.	Slag Rate	Top Pres.	Hot Metal Production	Sinter Rate	Iron Ore Rate	Lime Stone	Coke Rate
1017	4208	3.15	302	1.86	3608	1287	329	0	561
1004	4491	3.15	263	1.89	4786	1132	290	0	485
1000	4150	3.20	296	1.79	3855	1272	325	0	544
1000	4400	3.15	322	1.79	3696	1393	317	0	575
1000	4415	3.25	312	1.90	4041	1372	312	0	574
1000	4397	3.20	321	1.79	4010	1273	268	11	538
1000	4443	3.34	286	1.95	4259	1260	259	7	528
1010	4435	2.87	338	1.86	3675	1341	285	5	562
1004	4269	2.94	353	1.73	3741	1411	313	0	592
1008	4411	3.02	299	1.81	4601	1176	265	0	501

Chapter 7

Modeling Techniques Used for Coke Rate Prediction

7.1 Introduction

In the present work modeling techniques employed for coke rate prediction are simple regression, multiple linear regression, polynomial regression which are discussed in detail in literature [46][47]. Also fuzzy regression, fuzzy-GA regression, neural networks have been for coke rate prediction.

7.2 Simple Multiple and Polynomial Regression

In terms of a more generalised representation [48], if the dependent variable y is influenced by n independent variables $x_1, x_2, \ldots, x_n$ and has $m+1$ parameters or coefficients $A_0, A_1, \ldots, A_m$ then,

$$y = f(x_1, x_2, \ldots, x_n, A_0, A_1, \ldots, A_m) \tag{7.1}$$

Three possible models are:

1. If y is linear with respect to both independent variables and coefficients, the simple relation is,

$$y = A_0 + A_1x_1 + A_2x_2 + \cdots + A_nx_n \tag{7.2}$$

2. If y is linear with respect to parameters but nonlinear with respect to the independent then in case ofone independent variable x,

$$y = A_0 + A_1x + A_2x^2 + \cdots + A_nx^n \tag{7.3}$$

3. The relationship between y and x may be very complex. When y is non-linear with respect to both parameters and independent variables could be represented as,

$$y = e^{A_1x_1} + e^{A_2x_2} \tag{7.4}$$

Only those cases which have a linear relationship with respect to coefficients come under the category of linear regression; variables may or may not be linear with respect to the independent variables. If y is linear with respect to independent variable also then it is called simple linear regression (equation 7.2). The simple linear regression, however, is not always applicable and a curve may better fit the data. For such cases, the least square analysis can be easily extended to fit the data to an nth degree polynomial (equation 7.3). When y is a function of two or more variables, the simple linear regression is usually referred to as "multiple linear regression".

Stepwise linear regression can be used to eliminate some terms from the regression model equation (7.2, 7.3 or 7.4). It accomplishes this either by starting from a model

with no terms and proceeding forward, or by starting with a model containing all terms and proceeding backward. At each step, some criterion, such as adjusting the coefficient of determination (R^2) is used, to add or delete the predictor variables. At each step it considers both adding and deleting each predictor, until it reaches a point where no addition or deletion improves the model any further. In this work, standard routine RSTEP from IMS Library [49] has been used for stepwise addition or deletion of variables (see appendix D.6).

7.3 Non-linear Regression Using Neural Networks

Artificial neural networks (ANN) are being used frequently in problems of modeling. An artificial neural network mimics the way the human brain works. A neural net is a network of simple computing units called *neurons*. Fundamentals of ANN are amply described in literature [50][51][52].

A neural net can adapt to a problem/situation (or data) by changing their structure which is represented by the weights associated with the neuron-neuron connection. The main characteristics of this network to be used in the modeling are optimization and dynamic self-organization. Most commonly used algorithm in neural networks is Back Propagation Algorithm (or BPA). BPA has been used in modeling various processes in the iron and steel industry [53][54][55][56].

Neural networks has been used to carry out non-linear regression [57][58]. Since BPA also optimizes/reduces the error in the actual to predicted values by adjusting the weights of the network. Basically it follows the least square method of regression, using a nonlinear function. A comparison is shown in Table 7.1 below:

A common representation of a neural network is shown in Figure 7.1.

A neural network model more similar to statistical model is shown in Figure 7.2.

Table 7.1: A Comparison Between Neural Networks and Statistical Regression

Neural Networks	Statistics
Weights	Coefficients
Bias term	Constant term or Intercept
Inputs	Independent variables
Output	Dependent variables
Training/Learning	Coefficient estimation
Sigmoidal function	a nonlinear regression model e. g., $\sigma^{\star}(x) = (1 + e^{-x})^{-1}$
Radial Basis function	another nonlinear regression model; Gaussian pdf.

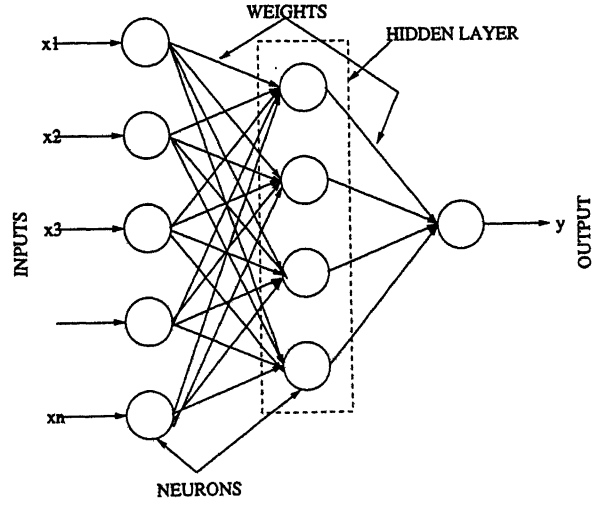


Figure 7.1: Artificial Neural Network

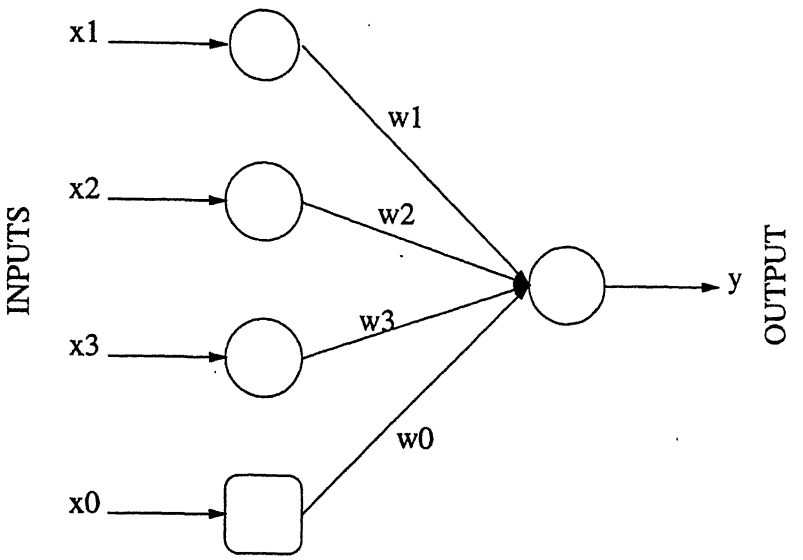


Figure 7.2: Regression Neural Network

This is a model of regression in three variables x_1, x_2 and x_3. The weights w_0, w_1, w_2 and w_3 are the coefficients of linear regression. We can represent the regression model as

$$y = \sigma^*(w_0 + w_1x_1 + w_2x_2 + w_3x_3) \tag{7.5}$$

where,

σ^* denotes the sigmoidal function (a bounded monotonic contineous function see Figure 7.3). $\sigma^*(x) = \frac{1}{(1+e^{-x})}$

The network uses non-linear least squares (NLLS) to estimate the parameters of the model, minimizing the residual sum of squares. This coefficient/ parameter estimation is called training of the neural network.

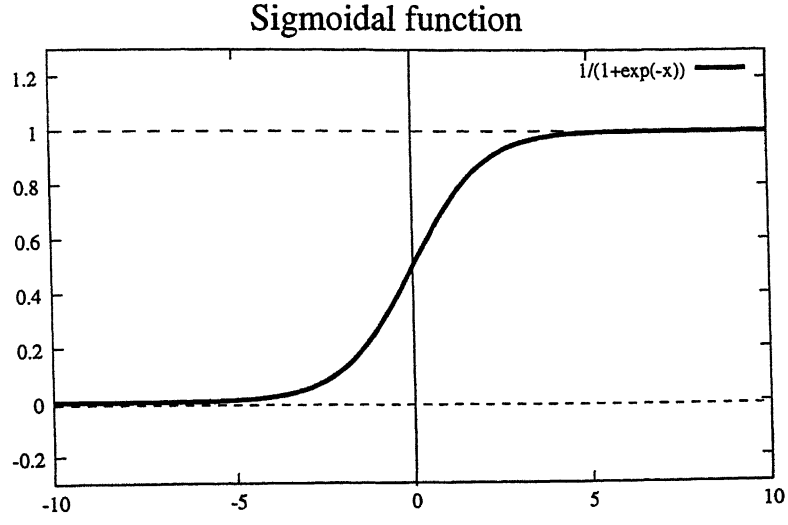


Figure 7.3: Sigmoidal Function

7.4 Fuzzy Regression

Fuzzy Regression technique differs from the conventional regression as follows. In conventional regression, (discussed in section 7.1) the difference between observed and estimated/calculated value, called observational error, is considered to be a random variable. It is probalistic in nature. In fuzzy regression the difference between observed and estimated/calculated values is assumed to be due to inherent ambiguity present in the system. The output value for a specific input values is thus assumed to be a range of possible values and **not** an exact or crisp value as it happens in case of normal conventional regression analysis. In other words, fuzzy regression is possiblistic in nature. Also coefficients used in fuzzy regression are fuzzy functions or numbers. A linear fuzzy regression model is of the form as shown in equation 7.6,

$$\tilde{y} = f(x, \tilde{A}) \tag{7.6}$$

It can be rewritten as,

$$\tilde{y} = \tilde{A}_1 x_1 + \tilde{A}_2 x_2 + \cdots + \tilde{A}_n x_n \tag{7.7}$$

where,

$\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_n$ are fuzzy coefficients and $\tilde{\Pi}$ is a fuzzy number.

7.4.1 Fuzzy number representation

A fuzzy number, as shown in Figure 7.4, is represented as a center-point or mid-point (p_i) and its spread (c_i). Thus representation of any fuzzy number is (p_i, c_i). So,

$$\tilde{A}_i = (p_i, c_i) \tag{7.8}$$

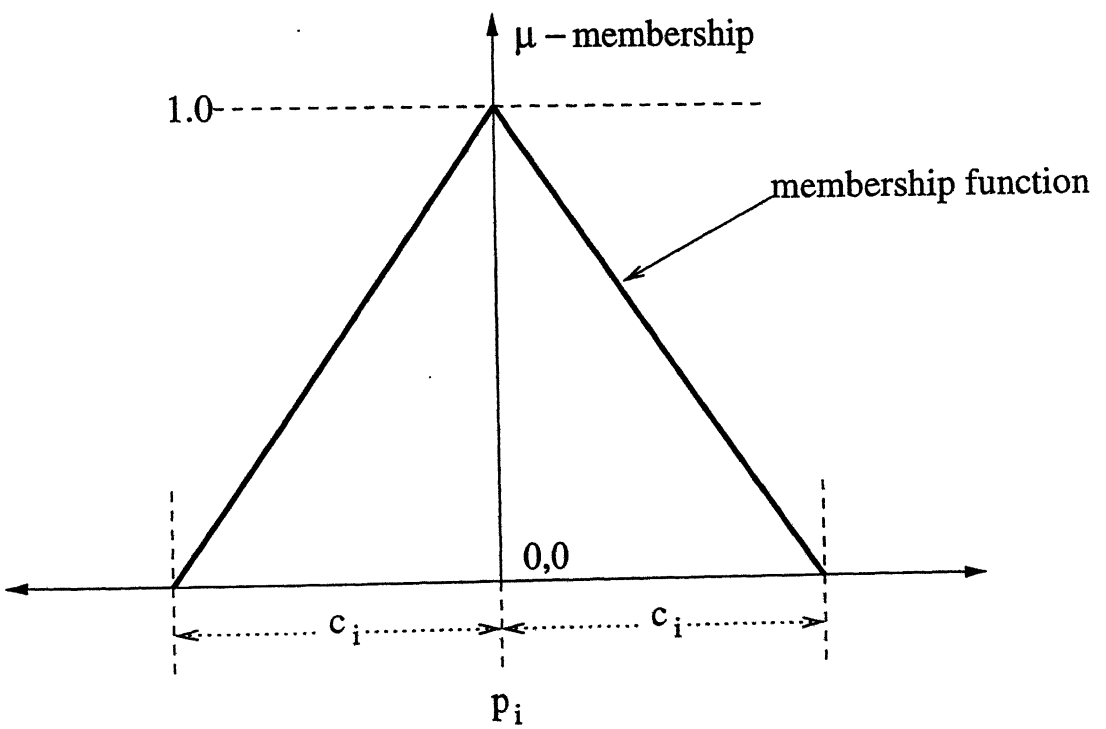


Figure 7.4: A fuzzy number representation

7.4.2 Procedure for Fuzzy Regression Using Linear Programming

The procedure for fuzzy regression using linear programming as described below has been adapted from the work of Ross [59].

Consider the data as shown in Table 6.1. Usually a data set is divided into two parts, such that alternate data are used for training and testing. Here are I am using full data 182 for finding coefficients (training) and also for testing.

We know that, mathematically,

$$\tilde{y} = \tilde{A}_1 x_1 + \tilde{A}_2 x_2 + \cdots + \tilde{A}_n x_n \tag{7.9}$$

Using equation 7.8, the model equation can be written as,

$$\tilde{y} = (p_1, c_1)x_1 + (p_2, c_2)x_2 + \cdots + (p_n, c_n)x_n \tag{7.10}$$

$$\tilde{y} = \sum_{i=1}^{n} (p_i, c_i)x_i \tag{7.11}$$

the membership function for y as defined by Ross [60], is,

$$\mu_y = \begin{cases} \max\left(\min\left[\mu_{A_i}\right]\right), & \{A \,|y = f\,(x, A)\,\} \neq \phi \\ 0, & otherwise \end{cases}$$

also, the generalised membership function could be written as,

$$\mu_{A_i} = \begin{cases} 1 - \frac{|p_i - c_i|}{c_i}, & (p_i - c_i) \leq x_i \leq (p_i + c_i) \\ 0, & otherwise \end{cases}$$

using above equation, we get,

$$\mu_{y_i} = \begin{cases} 1 - \frac{|y_i - \sum_i^n p_i x_i|}{\sum_i^n c_i}, & x_i \neq 0 \\ 1, & x_i = 0, \quad y_i = 0 \\ 0, & x_i = 0, \quad y_i \neq 0 \end{cases}$$

Tanaka [61] has used linear programming to find the solution for regression model. Now the objective of regression model is to determine the optimum parameters $\tilde{A}^*$ such that fuzzy output set, which contains y_i, is associated with a membership value greater than h,

$$\mu_{y_i} \geq h \qquad i = 1, 2, \ldots, n \tag{7.12}$$

As h increases the fuzziness of output increases. The corresponding values of spread and mid-point also vary. h is set by the user. Generally, $h = 0.5$ is taken.

In regression we find fuzzy coefficients that minimize spread of fuzzy output for all data sets.

The objective function to be minimized

$$Obj = \min \left[\sum_j^m \sum_i^n c_i x_{ij} \right] \tag{7.13}$$

and subject to two constraints (per data, so for n data $2n$ constraint. They are,

$$y_j \geq \sum_i^n p_i x_{ij} - (1-h) \sum_i^n c_i x_{ij} \tag{7.14}$$

$$y_j \leq \sum_i^n p_i x_{ij} + (1-h) \sum_i^n c_i x_{ij} \tag{7.15}$$

Using values from Table 6.1, the objective function to be minimized becomes,

$$Obj = \min[c_0 + c_1(x_{11} + x_{12} + \cdots + x_{nm}) + \cdots + c_n(x_{11} + x_{12} + \cdots + x_{nm})] \quad (7.16)$$

subject to constraints,

$$y_j \geq [p_0 + p_1 x_{1j} + \cdots + p_n x_{nj}] - (1-h)[c_0 + c_1 x_{1j} + \cdots + c_n x_{nj}] \quad (7.17)$$

$$y_j \leq [p_0 + p_1 x_{1j} + \cdots + p_n x_{nj}] + (1-h)[c_0 + c_1 x_{1j} + \cdots + c_n x_{nj}] \quad (7.18)$$

constraints for $j = 1, n$ where n = number of data.

The objective function given in equation 7.16 using data from Table 6.1 (having 9 independent and 1 dependent variables) gets transformed to equation 7.19,

$$\begin{aligned} Obj = \min [&c_0 + 187084.00 \times c_1 + 766281.00 \times c_2 + 535.66 \times c_3 + 58183.00 \times c_4 \\ &+305.14 \times c_5 + 696157.00 \times c_6 + 233829.00 \times c_7 + 53872.00 \times c_8 \\ &+456.00 \times c_9] \end{aligned} \quad (7.19)$$

The corresponding constraint equations for first data are shown below (equations 7.20 and 7.21). Such 364 constraint equations are generated ($2 \times 182 = 364$).

$$\begin{aligned} y_1 \geq [&p_0 + 1050.00 \times p_1 + 4250.00 \times p_2 + 3.00 \times p_3 + 319.00 \times p_4 \\ &1.70 \times p_5 + 4001.00 \times p_6 + 1168.00 \times p_7 + 379.00 \times p_8 + 9.00 \\ &\times p_9] - [c_0 + 525.00 \times c_1 + 2125.00 \times c_2 + 1.50 \times c_3 + 159.50 \end{aligned}$$

$$\times c_4 + 0.85 \times c_5 + 2000.50 \times c_6 + 584.00 \times c_7 + 189.50 \times c_8 + 4.50 \times c_9] \quad (7.20)$$

$$y_1 \leq [p_0 + 1050.00 \times p_1 + 4250.00 \times p_2 + 3.00 \times p_3 + 319.00 \times p_4 + 1.70 \times p_5 + 4001.00 \times p_6 + 1168.00 \times p_7 + 379.00 \times p_8 + 9.00 \times p_9] + [c_0 + 525.00 \times c_1 + 2125.00 \times c_2 + 1.50 \times c_3 + 159.50 \times c_4 + 0.85 \times c_5 + 2000.50 \times c_6 + 584.00 \times c_7 + 189.50 \times c_8 + 4.50 \times c_9] \quad (7.21)$$

Fuzzy regression using linear programming (LP) has been explained by Tanaka et al [61]. They have used linear programming to find the values of $p_0, p_1, \ldots, p_n$ and $c_0, c_1, \ldots, c_n$ for the regression model using standard NAG routine E04MBF [62] (see Appendix D.5).

7.4.3 Procedure for Fuzzy Regression Using GA

When linear programming is used as an optimization technique, even a slight non-linearity in the system may lead to a deviation at lower and upper bounds of data (see Figure 7.5) in most of the cases. A sample plot showing deviation at lower and upper bounds of data in prediction of silicon content of hot metal taken from my work on silicon content prediction [63] is given as an example in Figure 7.5. In order to account for the non-linearity, GA has been used in the present work to get the near-optimum values of fuzzy coefficients (see Table 8.8). GA has been found to be better than fuzzy regression using linear programming.

After obtaining the values of coefficients, calculated values of y (from the model developed) are defuzzified to get the crisp values. For defuzzification maximum mem-

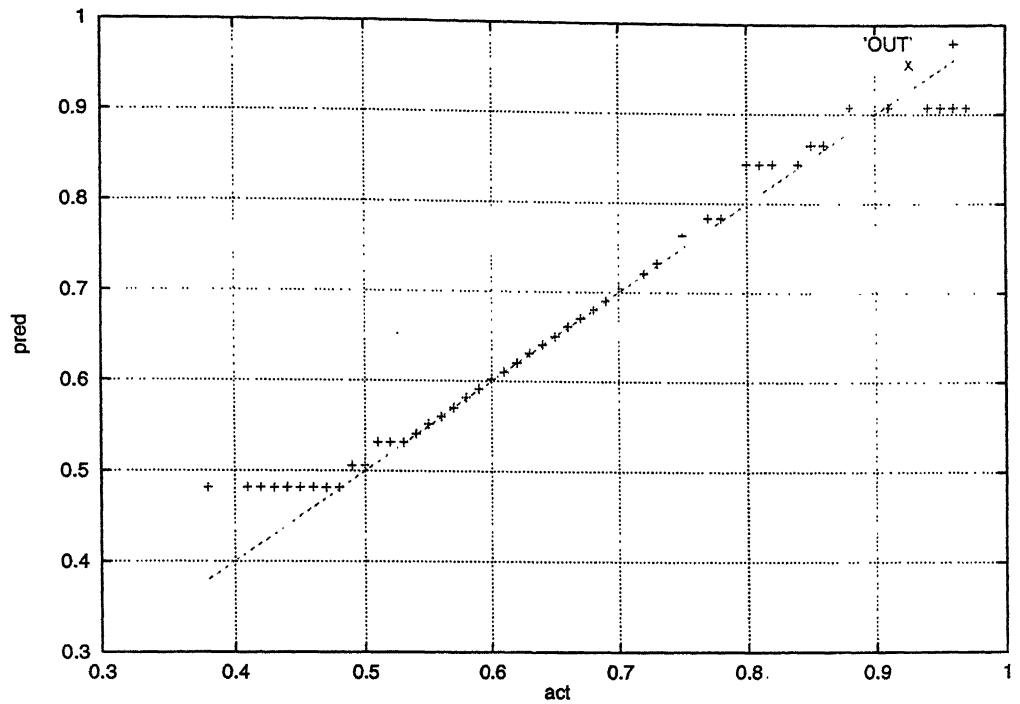


Figure 7.5: Deviation at Lower and Upper Bounds in Fuzzy Regression Using Linear Programming

bership function method [60] is used. The model returns values which are fuzzy numbers. In order to convert it back to a crisp value, we choose that value which is closest to the actual i.e., the value which has maximum membership. Another method that can be used for defuzzification is averaging, but it was not found suitable in the present problem.

7.4.4 Normal Regression Using GA

Normal regression using GA was also developed in this work. The task of fuzzy-GA regression on the data is to reduce the spread over the whole range of data.. From the figure 7.6 it is seen that with the value of $h = 0.5$ there is certain spread attached. If we make $h = 1.0$ then the spread becomes zero, and it becomes a normal regression. Thus normal regression becomes a special case of fuzzy regression.

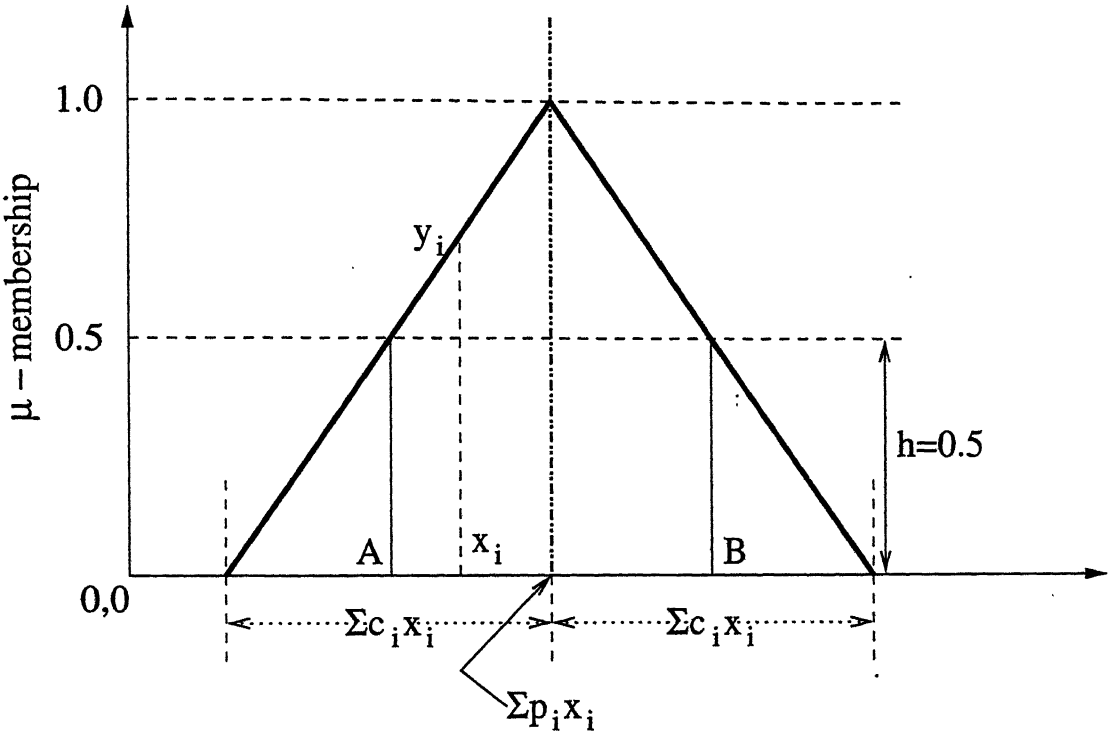


Figure 7.6: Representation of coefficient values using $h = 0.5$

Chapter 8

Coke Rate Prediction: Results and Discussion

8.1 Results

On the data given in section 6.1, coke rate ($kg/MTHM$) has been taken as dependent variable and the nine independent variables are: hot blast temperature ($°C$), cold blast flow (Nm^3), blast pressure ($atm.$), slag rate ($kg/MTHM$), top pressure ($atm.$), hot metal production (MT), sinter rate ($kg/MTHM$), iron ore rate ($kg/MTHM$) and lime stone consumption (MT). The results of different modeling techniques are presented below.

8.1.1 Results of Multiple Linear Regression

The multiple linear regression was carried out to predict coke rate (refer section 6.1) using standard NAG [62] routines G02BAF (appendix D.3), G02CGF (appendix D.4), G02CBF (appendix D.1) and G02CAF (appendix D.2) . The model coefficients obtained are listed in Table 8.1. The coke rate and the statistical analysis of actual

coke rate versus predicted coke rate is shown in Table 8.2. Correlation coefficient for both $y = mx$ and $y = mx + c$ plots are same 0.92 and standard error of estimation of coke rate are $\pm 12.9\,kg$ and $\pm 11.9\,kg$ respectively.

The plot in Figure 8.1 shows that there is a good agreement between actual and predicted coke rate values in the range of $490 - 580\,kg/MTHM$. The coefficient of the parameter "cold blast flow" is small, only -0.00273.

Table 8.1: Multiple Linear Regression (Coefficients)

S. No.	Coefficients	Value
1.	Constant	226.58468
2.	Hot blast temperature ($°C$)	-0.09329
3.	Cold blast flow (Nm^3)	-0.00273
4.	Blast pressure ($atm.$)	19.51266
5.	Slag rate ($kg/MTHM$)	0.49763
6.	Top pressure ($atm.$)	1.49129
7.	Hot metal production (MT)	-0.01193
8.	Sinter rate ($kg/MTHM$)	0.16039
9.	Iron ore rate ($kg/MTHM$)	0.13673
10.	Limestone consumption (MT)	-0.63051

Table 8.2: Multiple Linear Regression (Statistical Analysis)

$y = mx$		$y = mx + c$	
R	.92155	R	.9216
m	.99943	m	.8493
		c	81.0306
σ	12.93 kg	σ	11.95 kg
$F - value$	315466.0860	$F - value$	1014.0773

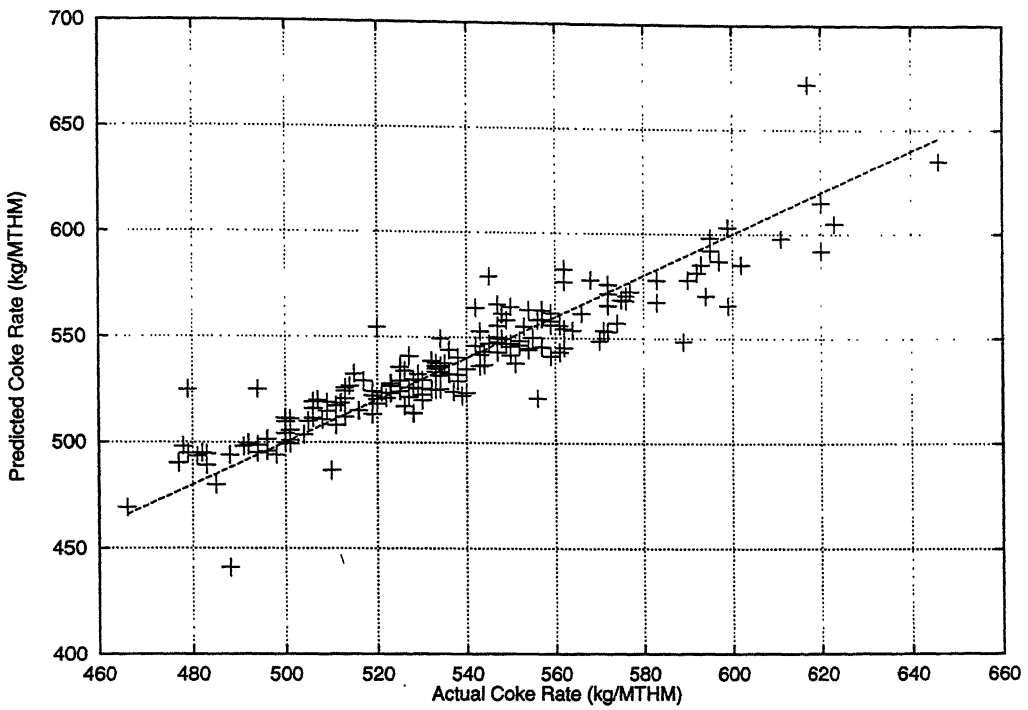


Figure 8.1: Actual Versus Predicted Coke Rate (Multiple Linear Regression)

8.1.2 Results of Stepwise Linear Regression

The IMS library [49] routine RSTEP (see appendix D.6) has been used to eliminate the variables which do not affect the regression model. The Cold blast flow and top pressure were eliminated. With rest of variables the multiple linear regression was carried out again. The coefficients obtained and statistical analysis of coke rate (actual versus predicted) are listed in Tables 8.3 and 8.4 respectively.

With respect to multiple linear regression, there is only little improvement in the correlation coefficient and standard error of estimation. Surprisingly, top pressure which had a coefficient of 1.491 in multiple linear regression is dropped in stepwise regression. The plot of actual versus predicted coke rate is shown in Figure 8.2 and is found similar to plot obtained in multiple linear regression (Figure 8.1).

Table 8.3: Stepwise Linear Regression (Coefficients)

S. No.	Coefficients	Value
1.	Constant	239.71905
2.	Hot blast temperature ($°C$)	-0.10457
3.	Blast pressure ($atm.$)	18.32539
4.	Slag rate ($kg/MTHM$)	0.49580
5.	Hot metal production (MT)	-0.01277
6.	Sinter rate ($kg/MTHM$)	0.15799
7.	Iron ore rate ($kg/MTHM$)	0.13650
8.	Limestone consumption (MT)	-0.66235

Table 8.4: Stepwise Linear Regression (Statistical Analysis)

$y = mx$		$y = mx + c$	
R	.92117	R	.9212
m	.99942	m	.8486
		c	81.4086
σ	12.95 kg	σ	11.97 kg
$F - value$	314003.8499	$F - value$	1008.5457

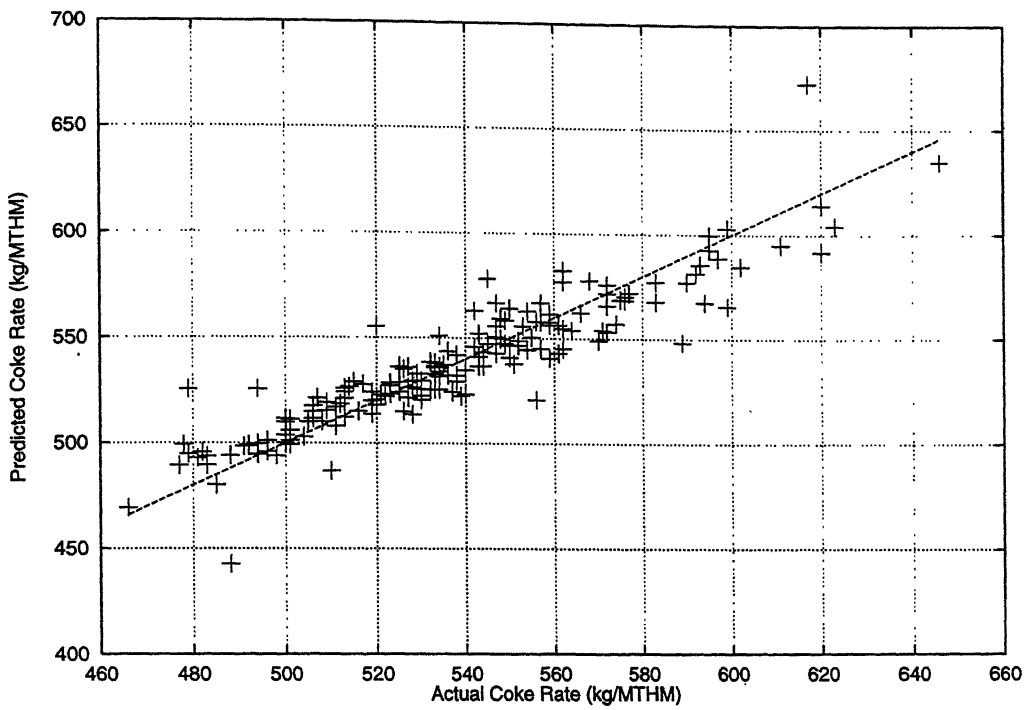


Figure 8.2: Actual Versus Predicted Coke Rate (Stepwise Linear Regression)

8.1.3 Results Using Neural Network

Singh and Deo [54] have used artificial neural networks to predict coke rate. The best correlation coefficient and standard deviation obtained were 0.95 and 13 kg respectively.

8.1.4 Results of Non-linear Regression Using Neural Network

In this work, non-linear regression was carried out using 9-1 neural network architecture. Since no hidden layer was present in the network which consisted of only input and output layers it ammounted to non-linear regression with exponential function. The statistics of the actual versus predicted values of the coke rate are listed in Table 8.5 below.

The correlation coefficient was 0.895 for both $y = mx$ and $y = mx + c$, and was

poor as compared to correlation coefficient (0.92) obtained by multiple and stepwise linear regression. The standard error of estimation is also more $\pm 15.2\, kg/MTHM$ as compared to $\pm 12.9\, kg/MTHM$ in case of $y = mx$ and $\pm 14.1\, kg/MTHM$ as compared to $\pm 11.9\, kg/MTHM$ for $y = mx+c$. Also it is seen (Figure 8.4) that the mean squared error decreases at a fast rate till 100 iterations, but afterwards the error reduces at a slower rate.

Table 8.5: Non-linear Regression Using Neural Network (Statistical Analysis)

$y = mx$		$y = mx + c$	
R	0.89531	R	0.8953
m	1.02092	m	0.8502
		c	92.1103
σ	15.20 kg	σ	14.13 kg
$F - value$	238218.6247	$F - value$	727.1757

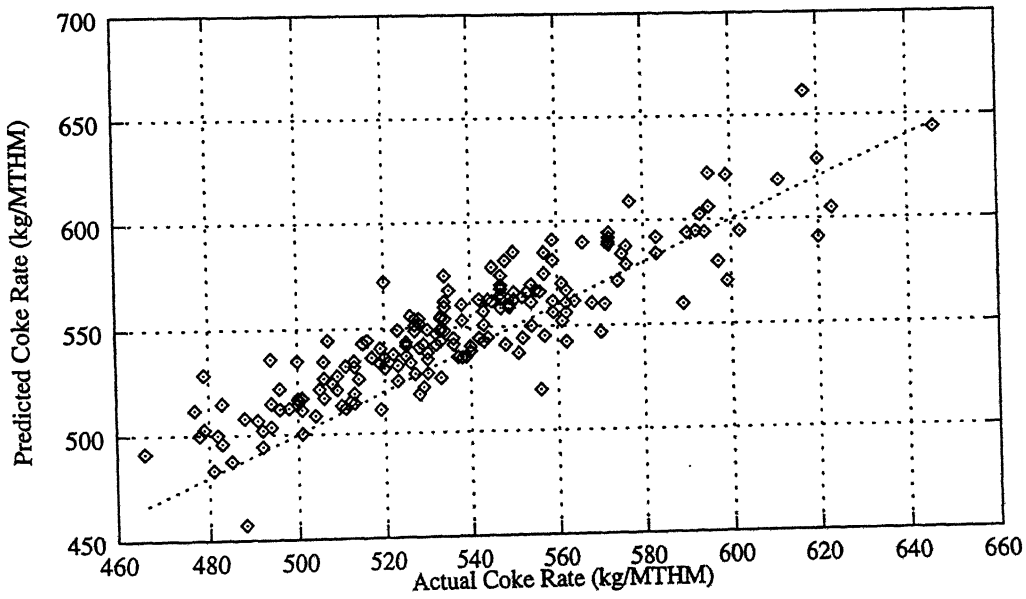


Figure 8.3: Actual Versus Predicted Coke Rate (Non-linear Regression Using Neural Network)

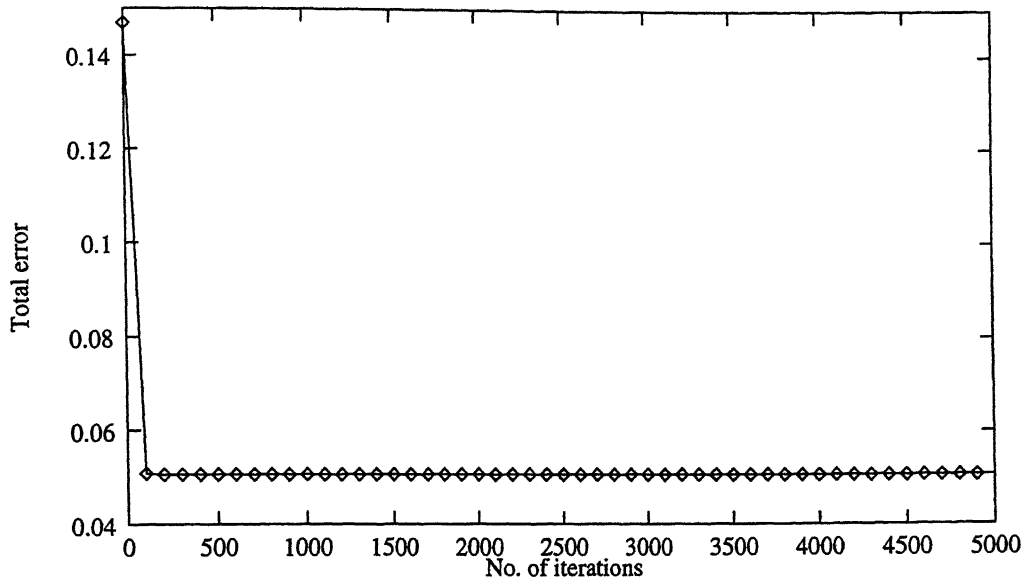


Figure 8.4: Plot between Number of Iterations and Mean Squared Error for Neural Network Used in Non-linear Regression

8.1.5 Results of Fuzzy Regression Using Linear Programming

Fuzzy regression was carried out using linear programming (standard NAG routine E04MBF [62] see appendix D.5). The correlation coefficient and standard error of estimates of coke rate were 0.99 and $\pm 2.2\, kg/MTHM$, respectively. As compared to the multiple linear regression (0.92), stepwise linear regression (0.92) and non-linear regression using neural network (0.89) models the correlation coefficient obtained by fuzzy regression using linear programming is highest (0.99). The standard error of estimate for coke rate is significantly low ($\pm 2.2\, kg/MTHM$) as compared to the earlier models. The actual and predicted values of coke rate are in good agreement over a larger range, $480 - 600\, kg/MTHM$ (Figure 8.5), where as earlier plots (Figures 8.1,8.2 and 8.3) show good prediction over a smaller range $490 - 580\, kg/MTHM$.

The spread values of the coefficients obtained are all zeros except for the constant (152.00).

Table 8.6: Fuzzy Regression Using Linear Programming (Fuzzy Coefficients)

S. No.	Fuzzy Coefficients	Mid-point	Spread
1.	Constant	0.5300000E+03	.1520000E+03
2.	Hot blast temperature ($°C$)	-0.1056677E+00	.0000000E+00
3.	Cold blast flow (Nm^3)	0.5295199E-02	.0000000E+00
4.	Blast pressure ($atm.$)	0.3980930E+02	.0000000E+00
5.	Slag rate ($kg/MTHM$)	0.2494775E+00	.0000000E+00
6.	Top pressure ($atm.$)	-0.6614309E+02	.0000000E+00
7.	Hot metal production (MT)	-0.4658993E-02	.0000000E+00
8.	Sinter rate ($kg/MTHM$)	0.4051000E-01	.0000000E+00
9.	Iron ore rate ($kg/MTHM$)	-0.7057104E-01	.0000000E+00
10.	Limestone consumption (MT)	-0.4068463E+01	.0000000E+00

Table 8.7: Fuzzy Regression Using Linear Programming (Statistical Analysis)

$y = mx$		$y = mx + c$	
R	.99790	R	.9979
m	1.00209	m	.9940
		c	4.3873
σ	2.217 kg	σ	2.206 kg
$F - value$	10062927.4072	$F - value$	39913.9899

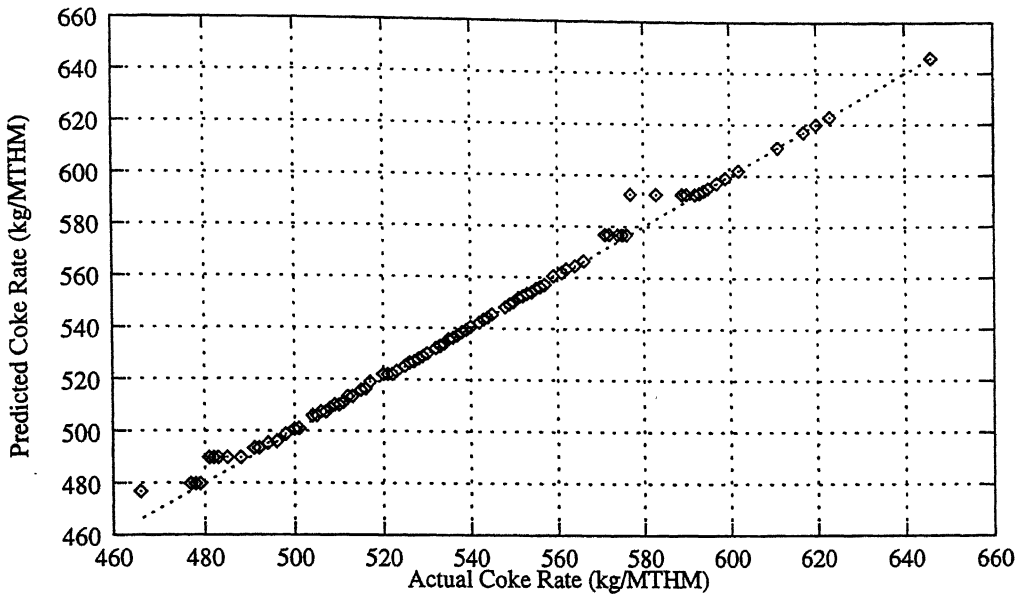


Figure 8.5: Actual Versus Predicted Coke Rate (Fuzzy Regression Using Linear Regression)

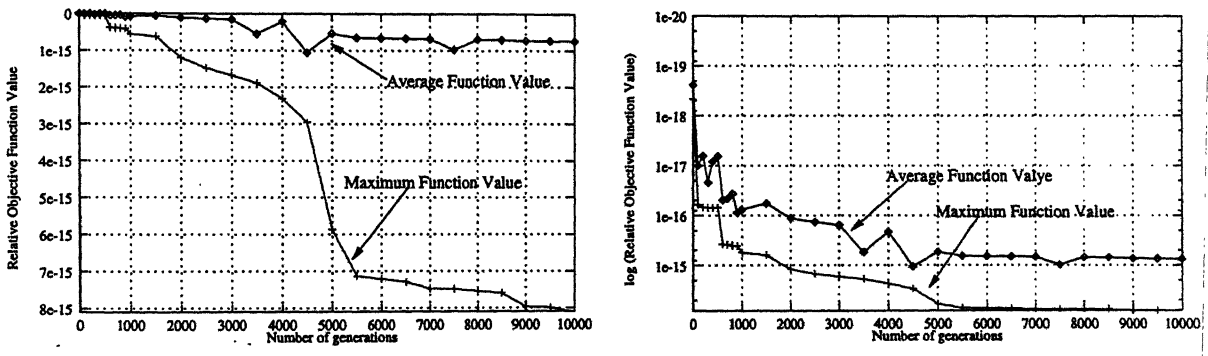
8.1.6 Results of Fuzzy-GA Regression

The fuzzy regression was carried out on the data using the new technique developed in this work. The coefficients obtained are listed in Table 8.8 and the statistics of actual versus predicted coke rate are given in the Table 8.9. Though the correlation coefficients in case of both fuzzy regressions, using linear programming and GA are nearly same (compare Tables 8.7 and 8.9), the GA shows better result if we look at the spread values of fuzzy coefficients obtained (compare Tables 8.6 and 8.8).

8.1.6.1 GA Parameters for Fuzzy-GA Regression

Carroll's Fortran code was used for optimizing the coefficient values. In the GA run, micro-GA (μGA) was used, with following parameters:

total number of parameters evaluated	20
total number of constraints	364
total binary string length	200
	(10 for each parameter)
population	11
(with 4 child strings kept for the next generation)	
mutation probability	0.00001
crossover probability	0.9
maximum generations	10000
Tournament selection, with uniform crossover and elitist selection is used.	
Upper bound for all parameters	1.0
Lower bound for mid-points parameters	-1.0
Lower bound for spread parameters	0.0



(a) (b)

Figure 8.6: Penalized Relative Objective Function Value at different generations (a) normal scale and, (b) in log scale

The Figure 8.6(a) shows the penalized relative objective function value convergence against the number of generations of GA run. The graph becomes more clearer when plotted on log scale (8.6(b)).

The correlation coefficient obtained for fuzzy-GA regression is 0.9999 and is the best out of all correlation coefficients obtained using various models for coke rate prediction. The standard error of estimates of coke rate are $\pm 0.40\, kg/MTHM$ and $\pm 0.39\, kg/MTHM$ for $y = mx$ and $y = mx + c$ plots. The values of standard error of estimate obtained by fuzzy-GA regression is very low as compared to those obtained in other models (fuzzy regression using linera programming $\pm 2.2\, kg/MTHM$; multiple and stepwise linear regression $\pm 12.9\, kg/MTHM$ and non-linear regression using neural network $\pm 15.2\, kg/MTHM$).

Another improvement in this model of fuzzy-GA regression over fuzzy regression using linear programming is in the spread values of the coefficients obtained. The spread of the constant is 0.567 as compared to 152.00 in case of fuzzy regression using linear programming. Also all the spread values are not zeros. Like fuzzy regression using linear programming the range of prediction is large $480 - 600\, kg/MTHM$ in case of fuzzy-GA rergression.

Table 8.8: Fuzzy-GA Regression (Fuzzy Coefficients)

S. No.	Fuzzy Coefficients	Mid-point	Spread
1.	Constant	0.6989E+00	0.5670E+00
2.	Hot blast temperature ($°C$)	-0.9775E-03	0.0000E+00
3.	Cold blast flow (Nm^3)	0.1075E-01	0.0000E+00
4.	Blast pressure ($atm.$)	0.9980E+00	0.2033E+00
5.	Slag rate ($kg/MTHM$)	0.6735E+00	0.0000E+00
6.	Top pressure ($atm.$)	0.8456E+00	0.1564E-01
7.	Hot metal production (MT)	-0.1662E-01	0.0000E+00
8.	Sinter rate ($kg/MTHM$)	0.1965E+00	0.0000E+00
9.	Iron ore rate ($kg/MTHM$)	0.2845E+00	0.0000E+00
10.	Limestone consumption (MT)	0.1574E+00	0.7918E-01

Table 8.9: Fuzzy-GA Regression (Statistical Analysis)

$y = mx$		$y = mx + c$	
R	.99992	R	.9999
m	1.00074	m	.9985
		c	1.2117
σ	0.40 kg	σ	0.395 kg
$F - value$	312316730.2882	$F - value$	1054829.1935

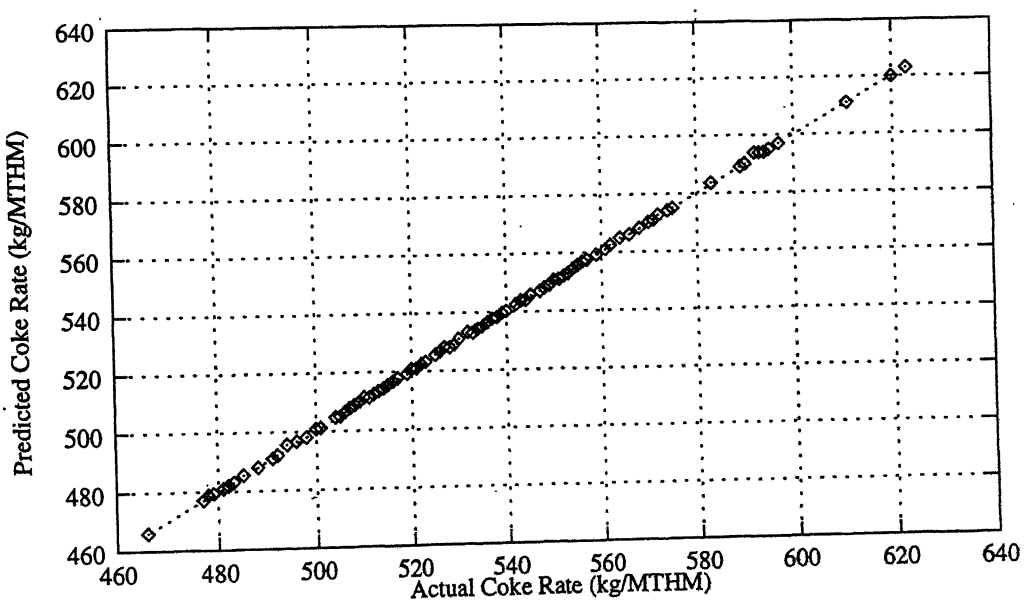


Figure 8.7: Actual Versus Predicted Coke Rate (Fuzzy-GA Regression)

8.1.7 Results of Normal Regression Using GA

An attempt was made to use GA to carry out the normal regression. When the spread values in the fuzzy model (see equation 7.10) become zero, the fuzzy regression model reduces to a noraml regression model.

GA was used to carry out the optimization of the coefficients using micro-GA (μGA) using following GA parameters:

total number of parameters evaluated	20
total number of constraints	364
total binary string length	100
	(5 for each parameter)
population	11
(with 4 child strings kept for the next generation)	
mutation probability	0.00001
crossover probability	0.9
maximum generations	20000
Tournament selection, with uniform crossover and elitist selection is used.	

The lower and upper bound set for different variables is listed in Table 8.10 below. The all spread values were set to zero.

The coefficients obtained by using GA are listed in Table 8.11 below. This method to carry out the normal regression did not give very good results as compared to least point estimate (compare Tables 8.2 and 8.12). The correlation coefficient in case of $y = mx$ and $y = mx + c$ is 0.84, which is low value as compared to other models discussed above. The standard error of estimates for coke rate was also poor $\pm 19.5\, kg/MTHM$.

Table 8.10: Lower and Upper Bounds for Different Variables

Variable	Lower bound	Upper bound
Constant	-250.0	250.0
Hot blast temp.	-1.0	1.0
Cold blast flow	-1.0	1.0
Blast press.	-25.0	25.0
Slag rate	-1.0	1.0
Top press.	-2.0	2.0
Hot metal prod.	-1.0	1.0
Sinter rate	-1.0	1.0
Iron ore rate	-1.0	1.0
Limestone	-1.0	1.0

Table 8.11: Normal Regression Using GA (Coefficients)

S. No.	Coefficients	Value
1.	Constant	0.1210E+03
2.	Hot blast temperature ($°C$)	-.3226E-01
3.	Cold blast flow (Nm^3)	0.3226E-01
4.	Blast pressure ($atm.$)	0.2339E+02
5.	Slag rate ($kg/MTHM$)	0.8065E+00
6.	Top pressure ($atm.$)	-.1097E+01
7.	Hot metal production (MT)	-.3226E-01
8.	Sinter rate ($kg/MTHM$)	0.9677E-01
9.	Iron ore rate ($kg/MTHM$)	-.3226E-01
10.	Limestone consumption (MT)	-.1000E+01

Table 8.12: Normal Regression Using GA (Statistical Analysis)

$y = mx$		$y = mx + c$	
R	.84379	R	.8438
m	.99936	m	.9223
		c	41.6005
σ	19.70 kg	σ	19.59 kg
$F - value$	135757.4553	$F - value$	444.9681

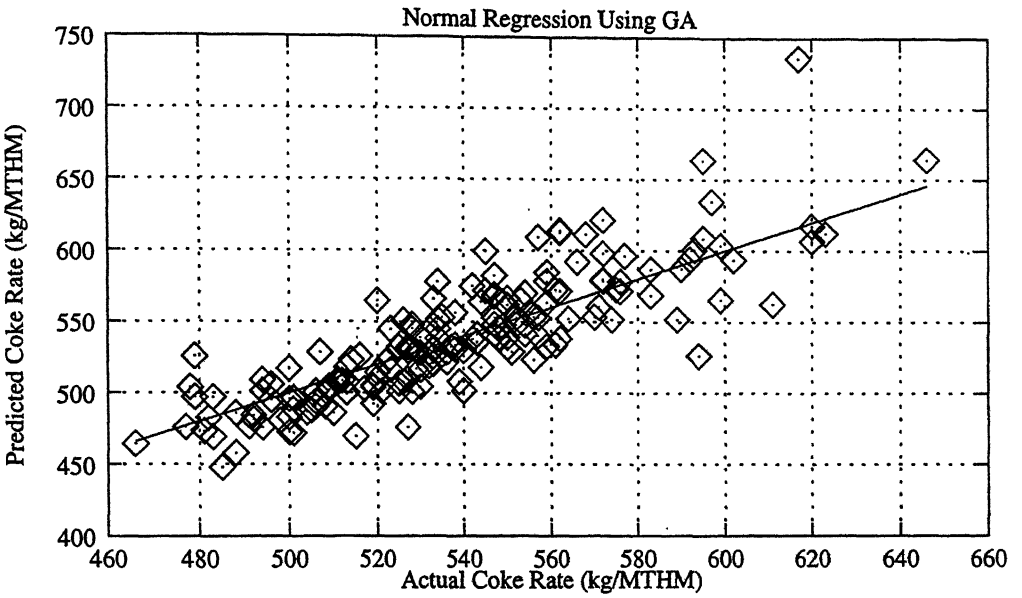


Figure 8.8: Actual Versus Predicted Coke Rate (Normal Regression Using GA)

Chapter 9

Conclusions

9.1 Coke Blend Optimization

On the basis of Figure 5.4 (comparison between the actual and the graph modeled using Fuzzy Associative Memory) it is concluded that FAM could be used for digitalizing such a complex graph which is otherwise difficult to be modeled by any other curve fitting technique such as, non-linear least square method etc..

The minimum cost obtained is $37.04 by a blend of coals comprising of Maple Creek, Riverside Sewell and Maben, but the sulfur constaint is not satisfied.

The maximum cost obtained is $42.42 by a blend of coals comprising of Terry Eagle, Riverside Sewell and Maben, with all the constaints satisfied.

The blend of coals, which satisfies all the constraints at a minimum cost ($39.10), comprises of coals Maple Creek, Amburgy, Riverside Sewell and Maben.

9.2 Coke Rate Prediction

Of all the modeling techniques used for coke rate prediction viz. multiple linear regression (correlation coefficient 0.9216; standard error of estimate $\pm 11.95\, kg/MTHM$), stepwise regression (correlation coefficient 0.9212; standard error of estimate $\pm 11.97\, kg/MTH$ nonlinear regression using neural networks (correlation coefficient 0.8953; standard error of estimate $\pm 14.13\, kg/MTHM$), fuzzy regression using linear programmimg (correlation coefficient 0.997; standard error of estimate $\pm 2.2\, kg/MTHM$), fuzzy-GA regression (correlation coefficient 0.9999; standard error of estimate $\pm 0.395\, kg/MTHM$) and normal regression using GA (correlation coefficient 0.8438; standard error of estimate $\pm 19.59\, kg/MTHM$); fuzzy-GA regression (a new technique developed in the present work) gave the best results having a correlation coefficient of 0.9999 and standard error of estimate $\pm 0.395\, kg/MTHM$ between the actual and predicted values.

Appendix A

Data for Coals

The coals used in the blending are:

1. Amburgy
2. Maben
3. Maple Creek
4. Riverside Sewell
5. Terry Eagle and
6. Wells

The data for these six coals used in the coal blending are given below.

A.1 Amburgy

Ash	5.98
Sulfur	0.66

Maceral Analysis with Mineral Matter		
Maceral	From Microscopic Examination (%)	Prorated (with Mineral Matter (%)
Vitrinite	76.00	73.41
Pseudovitrinite	0.00	0.00
Fusinite	4.80	4.64
Semifusinite	11.00	10.62
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	3.40	3.28
Oxyvitrinite	0.00	0.00
Exinite	4.80	4.64
Mineral Matter	—	3.41
Sum	100.00	100.00

V-Type	(%) in coal	(%) in Vitrinite
V7	16.00	16
V8	54.00	54
V9	30.00	30

% Reactives 81.59

% Inerts 18.41

Reactives Prorated as V-Types,

$$V7 = 81.59 \times \frac{16}{100} = 13.05$$

$$V8 = 81.59 \times \frac{54}{100} = 44.06$$

$$V9 = 81.59 \times \frac{30}{100} = 24.48$$

V-Type	Optimum Ratio	Strength Index
V7	3.0	3.0
V8	2.8	3.2
V9	2.6	3.5

Optimium Inerts : 29.40

Srtrength Index : 268.01

Inert Index : 0.63

Rank Index : 3.28

Predicted Stability : 49.69

A.2 Maben

Ash 5.91

Sulfur 0.72

Maceral Analysis with Mineral Matter		
Maceral	From Microscopic Examination (%)	Prorated (with Mineral Matter (%)
Vitrinite	73.40	71.91
Pseudovitrinite	0.00	0.00
Fusinite	5.20	5.02
Semifusinite	21.20	20.48
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	0.20	0.19
Oxyvitrinite	0.00	0.00
Exinite	0.00	0.00
Mineral Matter	—	3.39
Sum	100.00	100.00

V-Type	(%) in coal	(%) in Vitrinite
V15	4.00	4
V16	59.00	59
V17	36.00	36
V18	1.00	1

% Reactives 77.74

% Inerts 22.26

Reactives Prorated as V-Types,

$$V15 = 77.74 \times \frac{4}{100} = 3.11$$

$$V16 = 77.74 \times \frac{59}{100} = 45.87$$

$$V17 = 77.74 \times \frac{36}{100} = 27.99$$

$$v18 = 77.74 \times \frac{1}{100} = 0.78$$

V-Type	Optimum Ratio	Strength Index
V15	8.3	7.2
V16	10.8	7.3
V17	13.5	7.4
V18	16.1	7.5

Optimium Inerts : 6.74

Srtrength Index : 571.18

Inert Index : 3.30

Rank Index : 7.35

Predicted Stability : 41.87

A.3 Maple Creek

Ash 6.61

Sulfur 1.28

Maceral Analysis with Mineral Matter		
Maceral	From Microscopic Examination (%)	Prorated (with Mineral Matter (%)
Vitrinite	84.60	81.28
Pseudovitrinite	0.00	0.00
Fusinite	5.60	5.38
Semifusinite	6.60	6.34
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	0.40	0.38
Oxyvitrinite	0.00	0.00
Exinite	2.80	2.69
Mineral Matter	—	3.92
Sum	100.00	100.00

V-Type	(%) in coal	(%) in Vitrinite
V7	4.00	4
V8	75.00	75
V9	21.00	21

% Reactives 86.09

% Inerts 13.91

Reactives Prorated as V-Types,

$$V7 = 86.09 \times \frac{4}{100} = 3.44$$

$$V8 = 86.09 \times \frac{75}{100} = 64.56$$

$$V9 = 86.09 \times \frac{21}{100} = 18.08$$

V-Type	Optimum Ratio	Strength Index
V7	3.0	3.0
V8	2.8	3.2
V9	2.6	3.5

Optimium Inerts : 31.10

Srtrength Index : 283.44

Inert Index : 0.45

Rank Index : 3.29

Predicted Stability : 54.95

A.4 Riverside Sewell

Ash 3.96

Sulfur 0.73

Maceral Analysis with Mineral Matter		
Maceral	From Microscopic Examination (%)	Prorated (with Mineral Matter (%)
Vitrinite	77.40	75.59
Pseudovitrinite	0.00	0.00
Fusinite	3.60	3.52
Semifusinite	15.20	14.84
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	2.80	2.73
Oxyvitrinite	0.00	0.00
Exinite	1.00	0.98
Mineral Matter	——	2.34
Sum	100.00	100.00

V-Type	(%) in coal	(%) in Vitrinite
V11	1.00	1
V12	13.00	13
V13	58.00	59
V14	27.00	27

% Reactives 81.51

% Inerts 18.49

Reactives Prorated as V-Types,

$$V11 = 81.51 \times \frac{1}{100} = 0.82$$

$$V12 = 81.51 \times \frac{13}{100} = 10.70$$

$$V13 = 81.51 \times \frac{59}{100} = 47.76$$

$$V14 = 81.51 \times \frac{27}{100} = 22.23$$

V-Type	Optimum Ratio	Strength Index
V11	2.8	4.5
V12	3.4	5.1
V13	4.5	5.8
V14	6.2	6.5

Optimium Inerts : 17.69

Srtrength Index : 483.66

Inert Index : 1.05

Rank Index : 5.92

Predicted Stability : 59.02

A.5 Terry Eagle

Ash 6.71

Sulfur 0.67

Maceral Analysis with Mineral Matter		
Maceral	From Microscopic Examination (%)	Prorated (with Mineral Matter (%)
Vitrinite	82.00	78.88
Pseudovitrinite	0.00	0.00
Fusinite	3.60	3.46
Semifusinite	3.40	3.27
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	2.40	2.31
Oxyvitrinite	0.00	0.00
Exinite	8.60	8.27
Mineral Matter	——	3.81
Sum	100.00	100.00

V-Type	(%) in coal	(%) in Vitrinite
V8	21.00	21
V9	55.00	55
V11	24.00	24

% Reactives 88.24

% Inerts 11.76

Reactives Prorated as V-Types,

$$V7 = 88.24 \times \frac{21}{100} = 18.53$$

$$V8 = 88.24 \times \frac{55}{100} = 48.53$$

$$V9 = 88.24 \times \frac{24}{100} = 21.18$$

V-Type	Optimum Ratio	Strength Index
V7	2.8	3.2
V8	2.6	3.5
V9	2.6	4.0

Optimium Inerts : 33.35

Srtrength Index : 314.80

Inert Index : 0.35

Rank Index : 3.57

Predicted Stability : 59.29

A.6 Wells

Ash 5.59

Sulfur 0.88

Maceral Analysis with Mineral Matter		
Maceral	From Microscopic Examination (%)	Prorated (with Mineral Matter (%)
Vitrinite	74.20	71.78
Pseudovitrinite	0.00	0.00
Fusinite	4.00	3.87
Semifusinite	9.00	8.71
Macrinite	0.00	0.00
Semimacrinite	0.00	0.00
Micrinite	2.80	2.71
Oxyvitrinite	0.00	0.00
Exinite	10.00	9.67
Mineral Matter	——	3.26
Sum	100.00	100.00

V-Type	(%) in coal	(%) in Vitrinite
V7	1.00	1
V8	16.00	16
V9	55.00	55
V10	28.00	28

% Reactives 84.36

% Inerts 15.64

Reactives Prorated as V-Types,

$$V7 = 84.36 \times \frac{1}{100} = 0.84$$

$$V8 = 84.36 \times \frac{16}{100} = 13.50$$

$$V9 = 84.36 \times \frac{55}{100} = 46.40$$

$$V10 = 84.36 \times \frac{28}{100} = 23.62$$

V-Type	Optimum Ratio	Strength Index
V7	3.0	3.0
V8	2.8	3.2
V9	2.6	3.5
V10	2.6	4.0

Optimium Inerts : 31.97

Srtrength Index : 303.26

Inert Index : 0.49

Rank Index : 3.60

Predicted Stability : 58.37

Appendix B

Genetic Algorithms

B.1 Overview

GAs simulate the survival of the fittest among individuals over consecutive generation for solving a problem. Each generation consists of a population of character strings that are analogous to the chromosome that we see in a DNA (see figure B.1). Each individual represents a point in a search space and a possible solution. The individuals in the population are then made to go through a process of evolution.

GAs are based on an analogy with the genetic structure and behaviour of chromosomes within a population of individuals using the following foundations:

- Individuals in a population compete for resources and mates.
- Those individuals most successful in each 'competition' will produce more offspring than those individuals that perform poorly.
- Genes from 'good' individuals propagate throughout the population so that two good parents will sometimes produce offspring that are better than either parent.

- Thus each successive generation will become more suited to their environment.

B.1.1 Search Space

A population of individuals is maintained within search space for a GA, each representing a possible solution to a given problem. Each individual is coded as a finite length vector of components, or variables, in terms of the binary alphabet {0,1}. To continue the genetic analogy these individuals are likened to chromosomes and the variables are analogous to genes. Thus a chromosome (solution) is composed of several genes (variables). A fitness score is assigned to each solution representing the abilities of an individual to 'compete'. The individual with the optimal (or generally near optimal) fitness score is sought. The GA aims to use selective 'breeding' of the solutions to produce 'offspring' better than the parents by combining information from the chromosomes.

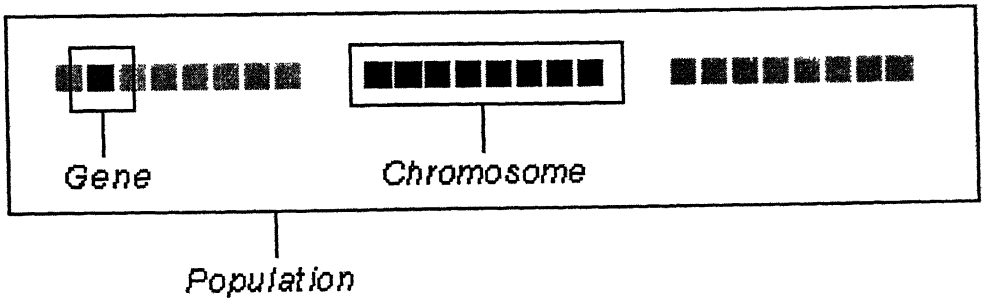


Figure B.1: A figure showing a gene, a chromosome and a population

The GA maintains a population of n chromosomes (solutions) with associated fitness values. Parents are selected to mate, on the basis of their fitness, producing offspring via a reproductive plan. Consequently highly fit solutions are given more opportunities to reproduce, so that offspring inherit characteristics from each parent. As parents mate and produce offspring, room must be made for the new arrivals since the population is kept at a static size. Individuals in the population die and are

replaced by the new solutions, eventually creating a new generation once all mating opportunities in the old population have been exhausted. In this way it is hoped that over successive generations better solutions will thrive while the least fit solutions die out.

New generations of solutions are produced containing, on average, more good genes than a typical solution in a previous generation. Each successive generation will contain more good 'partial solutions' than previous generations. Eventually, once the population has converged and is not producing offspring noticeably different from those in previous generations, the algorithm itself is said to have converged to a set of solutions to the problem at hand.

B.2 GA Operators

B.2.1 Selection Operator

The main idea behind having this selection operator is to give preference to better individuals, so that allowing them to pass on their genes to the next generation. The goodness of each individual depends on its fitness. And the fitness may be determined by an objective function.

B.2.2 Crossover Operator

The crossover operator is one operator that primarily distinguishes GA from other optimization techniques. Two individuals are chosen from the population using the selection operator. Then a crossover site along the bit strings is randomly chosen. The values of the two strings are exchanged up to this point, as shown in the example below.

Consider two strings $s1$ and $s2$

$$s1 = 0\ 0\ 0\ 0\ 0\ 0$$
$$s2 = 1\ 1\ 1\ 1\ 1\ 1$$

If the crossover point is 2, then,

$$s1 = 0\ 0 \mid 0\ 0\ 0\ 0$$
$$s2 = 1\ 1 \mid 1\ 1\ 1\ 1$$

The two new offsprings $s1'$ and $s2'$ created from this mating are,

$$s1' = 0\ 0\ 1\ 1\ 1\ 1$$
$$s2' = 1\ 1\ 0\ 0\ 0\ 0$$

They are put into the next generation of the population By recombining portions of good individuals, this process creates even better individuals. Another figure B.2 shows crossover below,

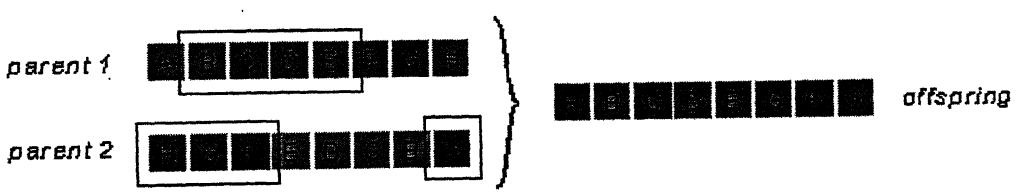


Figure B.2: Crossover Operation

B.2.3 Mutation Operator

This operator induces a random walk in the search space. With some low probability, called the mutation probability, a portion of the new individuals will have some

of their bits flipped (as shown in Figure B.3), i.e., 0 changed to 1 and vicé-versa. Its purpose is to maintain diversity within the population and inhibit premature convergence. Mutation and selection (without crossover) create a parallel, noise-tolerant, hill-climbing algorithms.

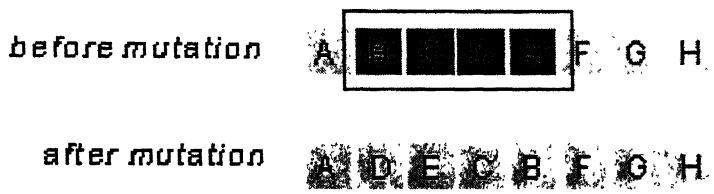


Figure B.3: Mutation Operation

B.3 Effects of Genetic Operators

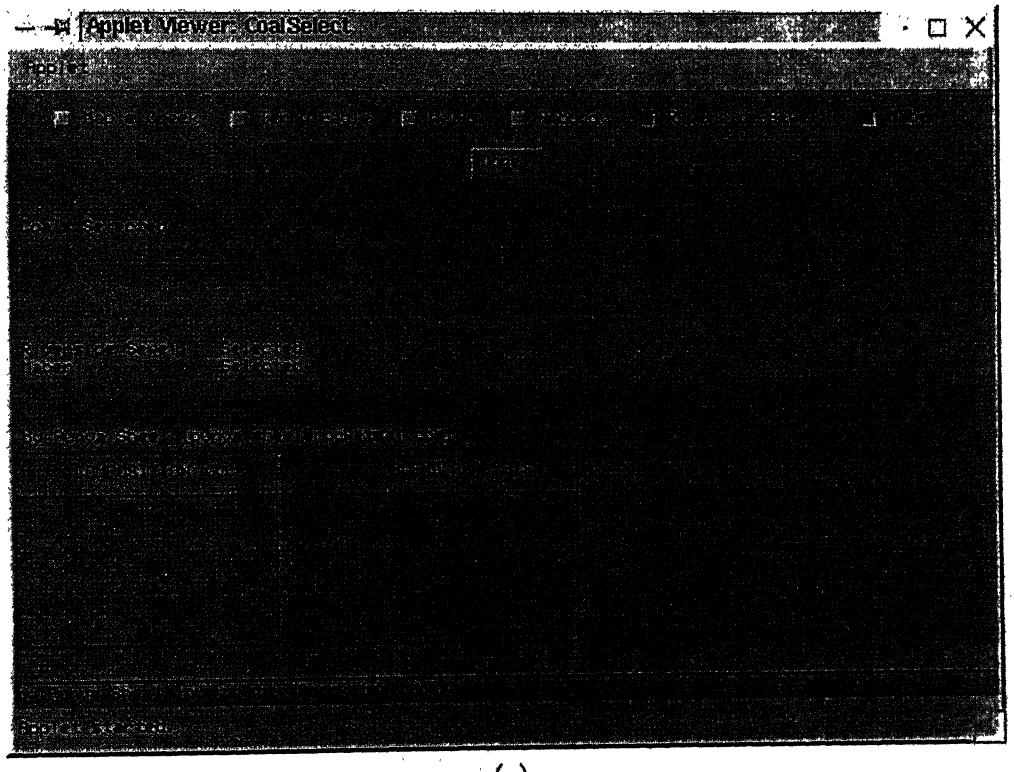
The effect of various operators alone and combined is as follows:

- Using selection alone tend to fill the population with copies of the best individual from the population.
- Using selection and crossover operators will tend to cause the algorithms to converge on a good but sub-optimal solution.
- Using mutation alone induces a random walk through the search space.
- Using selection and mutation creates a parallel, noise-tolerant, hill climbing algorithm.

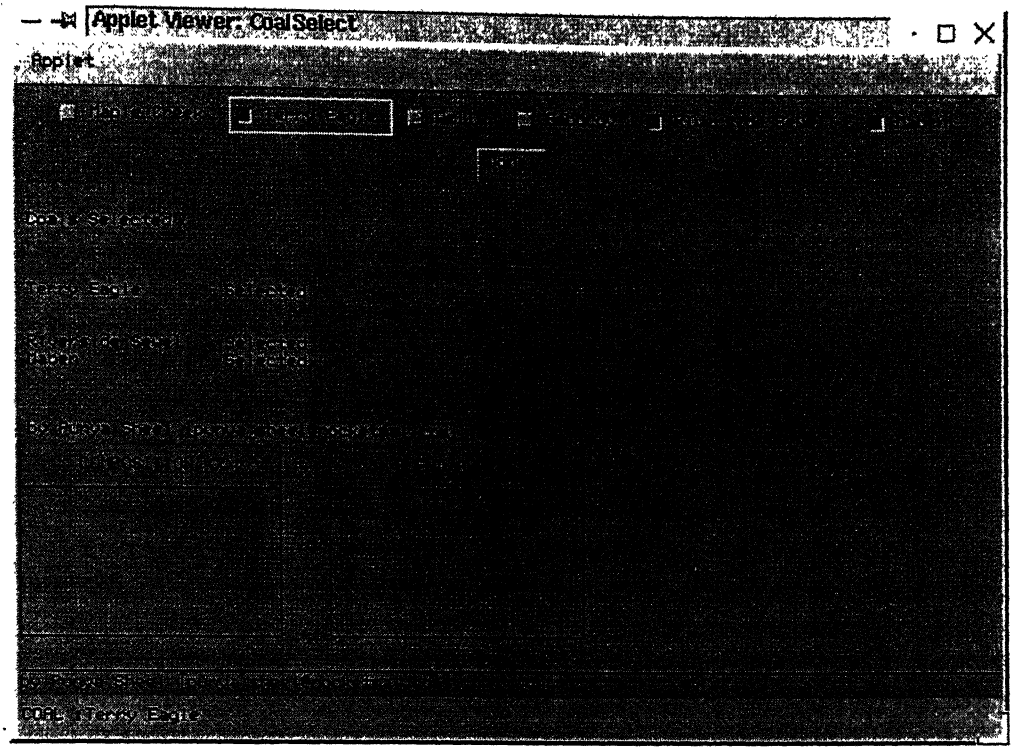
Appendix C

Java Applet for Coal Selection

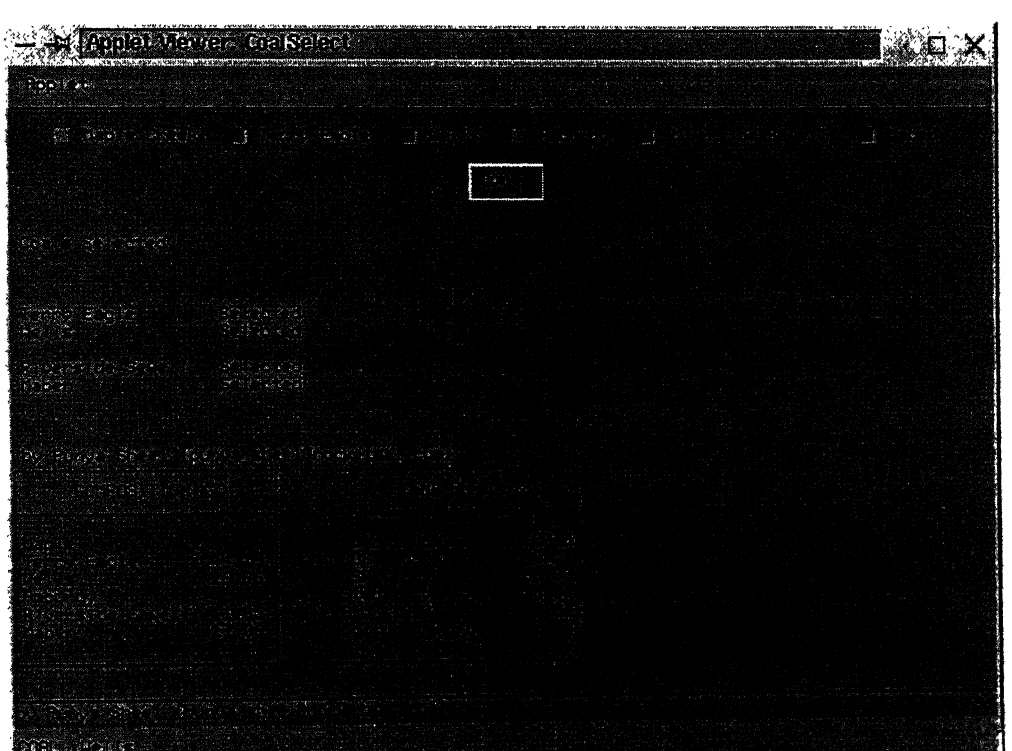
Figure C.1: Java Applet for Coal Selection Snapshots



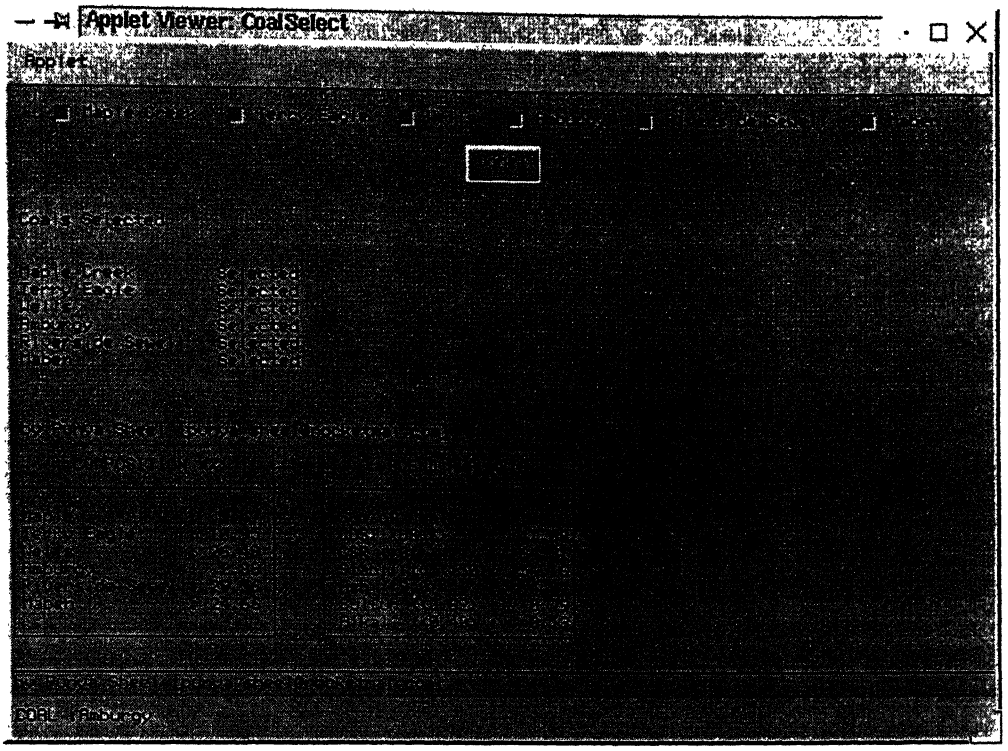
(a)


Applet Viewer: CoalSelect
Applet

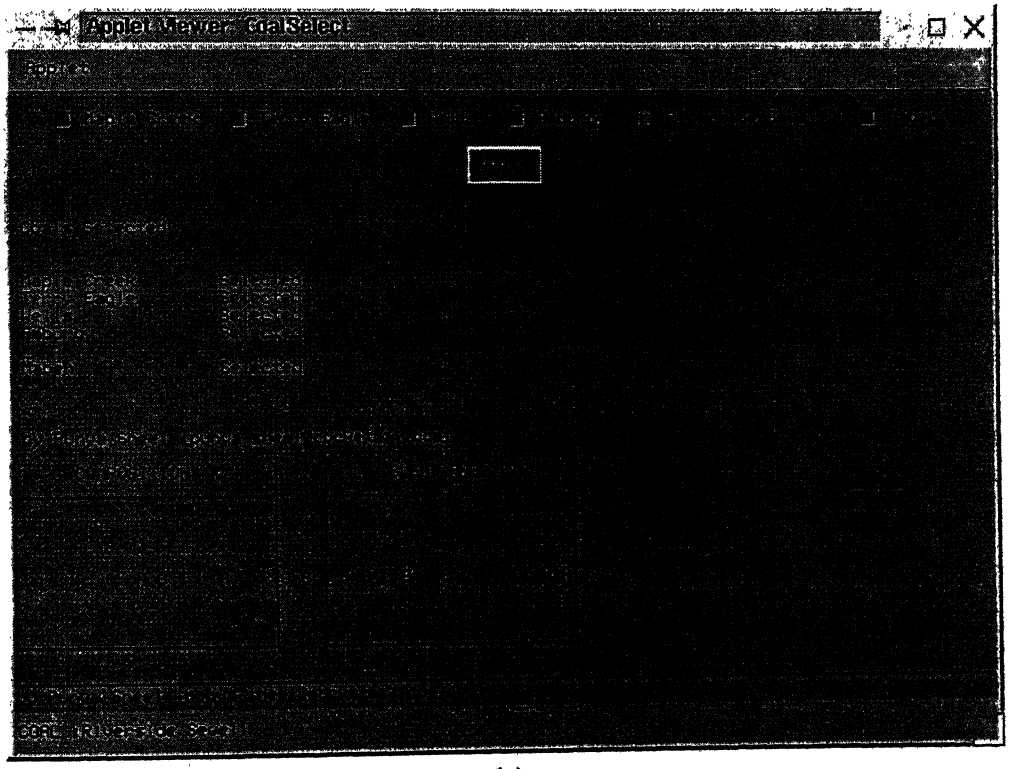
(b)


Applet Viewer: CoalSelect

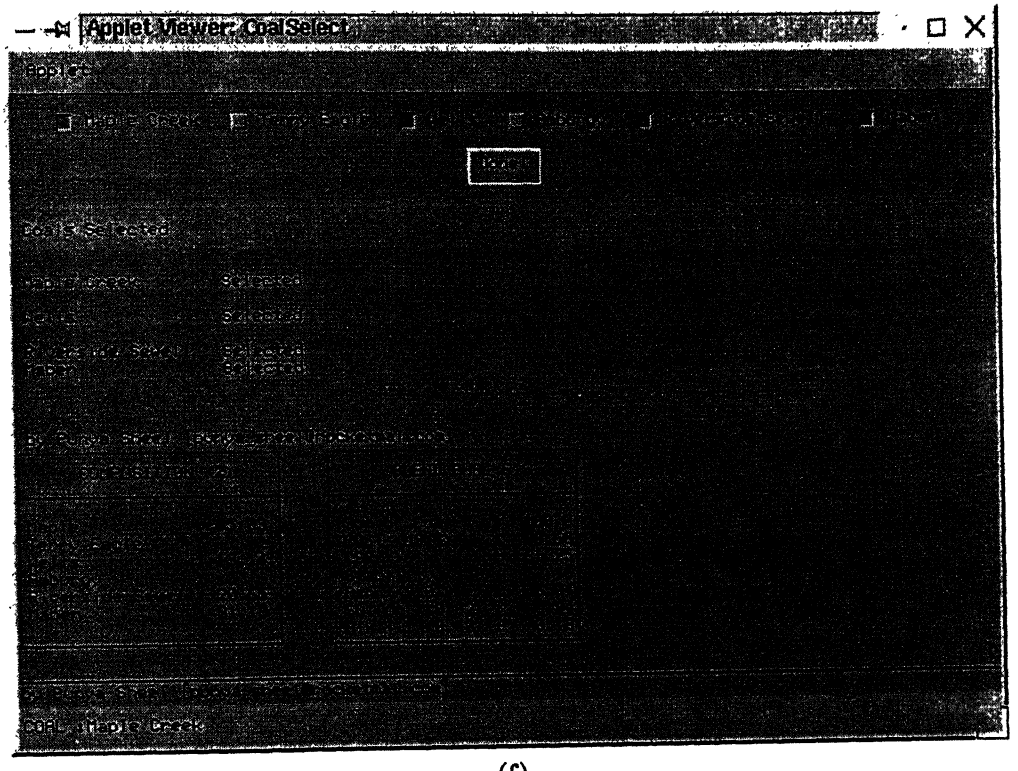
(c)


Applet Viewer: CoalSelect
Applet

(d)


Applet Viewer: CoalSelect

(e)



(f)

Appendix D

Standard FORTRAN Routines

D.1 NAG Routine G02CBF

Algorithm 1 Fortran Code for G02CBF [62]

```
*     G02CBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          N
      PARAMETER        (N=182)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL
*     .. Local Arrays ..
      DOUBLE PRECISION RESULT(20), X(N), Y(N)
*     .. External Subroutines ..
```

Appendix D

Standard FORTRAN Routines

D.1 NAG Routine G02CBF

Algorithm 1 Fortran Code for G02CBF [62]

```
*     G02CBF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          N
      PARAMETER        (N=182)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL
*     .. Local Arrays ..
      DOUBLE PRECISION RESULT(20), X(N), Y(N)
*     .. External Subroutines ..
```

```
      EXTERNAL         G02CBF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'G02CBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) (X(I),Y(I),I=1,N)
      WRITE (NOUT,*)
      WRITE (NOUT,*) ' Case      Independent      Dependent'
      WRITE (NOUT,*) 'number      variable        variable'
      WRITE (NOUT,*)
      WRITE (NOUT,99999) (I,X(I),Y(I),I=1,N)
      WRITE (NOUT,*)
      IFAIL = 1
*
      CALL G02CBF(N,X,Y,RESULT,IFAIL)
*
      IF (IFAIL.NE.0) THEN
         WRITE (NOUT,99998) 'Routine fails, IFAIL =', IFAIL
      ELSE
         WRITE (NOUT,99997)
     +     'Mean of independent variable                = ', RESULT(1)
         WRITE (NOUT,99997)
     +     'Mean of   dependent variable                = ', RESULT(2)
         WRITE (NOUT,99997)
     +     'Standard deviation of independent variable = ', RESULT(3)
         WRITE (NOUT,99997)
```

```
     +     'Standard deviation of   dependent variable = ', RESULT(4)
           WRITE (NOUT,99997)
     +     'Correlation coefficient                     = ', RESULT(5)
           WRITE (NOUT,*)
           WRITE (NOUT,99997)
     +     'Regression coefficient                      = ', RESULT(6)
           WRITE (NOUT,99997)
     +     'Standard error of coefficient               = ', RESULT(8)
           WRITE (NOUT,99997)
     +     't-value for coefficient                     = ', RESULT(10)
           WRITE (NOUT,*)
           WRITE (NOUT,*) 'Analysis of regression table :-'
           WRITE (NOUT,*)
           WRITE (NOUT,*)
     +'      Source         Sum of squares  D.F.    Mean square      F-val
     +ue'
           WRITE (NOUT,*)
           WRITE (NOUT,99996) 'Due to regression', (RESULT(I),I=12,15)
           WRITE (NOUT,99996) 'About  regression', (RESULT(I),I=16,18)
           WRITE (NOUT,99996) 'Total             ', (RESULT(I),I=19,20)
         END IF
         STOP
*
99999 FORMAT (1X,I4,2F15.4)
99998 FORMAT (1X,A,I2)
99997 FORMAT (1X,A,F10.5)
```

```
99996 FORMAT (1X,A,F14.4,F8.0,2F14.4)
      END
```

D.2 NAG Routine G02CAF

Algorithm 2 Fortran Code for G02CAF [62]

```
*     G02CAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          N
      PARAMETER        (N=182)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL
*     .. Local Arrays ..
      DOUBLE PRECISION RESULT(20), X(N), Y(N)
*     .. External Subroutines ..
      EXTERNAL         G02CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'G02CAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) (X(I),Y(I),I=1,N)
      WRITE (NOUT,*)
```

```
99996 FORMAT (1X,A,F14.4,F8.0,2F14.4)
      END
```

D.2 NAG Routine G02CAF

Algorithm 2 Fortran Code for G02CAF [62]

```
*     G02CAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          N
      PARAMETER        (N=182)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL
*     .. Local Arrays ..
      DOUBLE PRECISION RESULT(20), X(N), Y(N)
*     .. External Subroutines ..
      EXTERNAL         G02CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'G02CAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) (X(I),Y(I),I=1,N)
      WRITE (NOUT,*)
```

```
      WRITE (NOUT,*) ' Case      Independent      Dependent'
      WRITE (NOUT,*) 'number      variable         variable'
      WRITE (NOUT,*)
      WRITE (NOUT,99999) (I,X(I),Y(I),I=1,N)
      WRITE (NOUT,*)
      IFAIL = 1
*
      CALL G02CAF(N,X,Y,RESULT,IFAIL)
*
      IF (IFAIL.NE.0) THEN
         WRITE (NOUT,99998) 'Routine fails, IFAIL =', IFAIL
      ELSE
         WRITE (NOUT,99997)
     +     'Mean of independent variable                = ', RESULT(1)
         WRITE (NOUT,99997)
     +     'Mean of   dependent variable                = ', RESULT(2)
         WRITE (NOUT,99997)
     +     'Standard deviation of independent variable = ', RESULT(3)
         WRITE (NOUT,99997)
     +     'Standard deviation of   dependent variable = ', RESULT(4)
         WRITE (NOUT,99997)
     +     'Correlation coefficient                     = ', RESULT(5)
         WRITE (NOUT,*)
         WRITE (NOUT,99997)
     +     'Regression coefficient                      = ', RESULT(6)
         WRITE (NOUT,99997)
```

```
     +      'Standard error of coefficient              = ', RESULT(8)
            WRITE (NOUT,99997)
     +      't-value for coefficient                    = ', RESULT(10)
            WRITE (NOUT,*)
            WRITE (NOUT,99997)
     +      'Regression constant                        = ', RESULT(7)
            WRITE (NOUT,99997)
     +      'Standard error of constant                 = ', RESULT(9)
            WRITE (NOUT,99997)
     +      't-value for constant                       = ', RESULT(11)
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Analysis of regression table :-'
            WRITE (NOUT,*)
            WRITE (NOUT,*)
     +'      Source          Sum of squares  D.F.    Mean square      F-val
     +ue'
            WRITE (NOUT,*)
            WRITE (NOUT,99996) 'Due to regression', (RESULT(I),I=12,15)
            WRITE (NOUT,99996) 'About  regression', (RESULT(I),I=16,18)
            WRITE (NOUT,99996) 'Total             ', (RESULT(I),I=19,20)
          END IF
          STOP
*
99999 FORMAT (1X,I4,2F15.4)
99998 FORMAT (1X,A,I2)
99997 FORMAT (1X,A,F8.4)
```

```
99996 FORMAT (1X,A,F14.4,F8.0,2F14.4)
      END
```

D.3 NAG Routine G02BAF

Algorithm 3 Fortran Code for G02BAF [62]

```
*     G02BAF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          M, N, IA, ISSP, ICORR
      PARAMETER        (M=10,N=182,IA=N,ISSP=M,ICORR=M)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      DOUBLE PRECISION A(IA,M), AMEAN(M), CORR(ICORR,M), SSP(ISSP,M),
     +                 STD(M)
*     .. External Subroutines ..
      EXTERNAL         G02BAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'G02BAF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) ((A(I,J),J=1,M),I=1,N)
```

```
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'Number of variables (columns) =', M
      WRITE (NOUT,99999) 'Number of cases     (rows)    =', N
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Data matrix is:-'
      WRITE (NOUT,*)
      WRITE (NOUT,99998) (J,J=1,M)
      WRITE (NOUT,99997) (I,(A(I,J),J=1,M),I=1,N)
      WRITE (NOUT,*)
      IFAIL = 1
*
      CALL G02BAF(N,M,A,IA,AMEAN,STD,SSP,ISSP,CORR,ICORR,IFAIL)
*
      IF (IFAIL.NE.0) THEN
         WRITE (NOUT,99999) 'Routine fails, IFAIL =', IFAIL
      ELSE
         WRITE (NOUT,*) 'Variable   Mean    St. dev.'
         WRITE (NOUT,99996) (I,AMEAN(I),STD(I),I=1,M)
         WRITE (NOUT,*)
         WRITE (NOUT,*)
     +     'Sums of squares and cross-products of deviations'
         WRITE (NOUT,99998) (I,I=1,M)
         WRITE (NOUT,99997) (I,(SSP(I,J),J=1,M),I=1,M)
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Correlation coefficients'
         WRITE (NOUT,99998) (I,I=1,M)
```

```
         WRITE (NOUT,99997) (I,(CORR(I,J),J=1,M),I=1,M)
      END IF
      STOP
*
99999 FORMAT (1X,A,I3)
99998 FORMAT (1X,10I12)
99997 FORMAT (1X,I3,10F18.4)
99996 FORMAT (1X,I5,2F11.4)
      END
```

D.4 NAG Routine G02CGF

Algorithm 4 Fortran Code for G02CGF [62]

```
*     G02CGF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          K1, N, K, ISSP, ICORR, ICOEFF, IRINV, IC, IW
      PARAMETER        (K1=10,N=182,K=K1-1,ISSP=K1,ICORR=K1,ICOEFF=K,
     +                 IRINV=K,IC=K,IW=K)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J
*     .. Local Arrays ..
      DOUBLE PRECISION C(IC,K), COEFFT(ICOEFF,3), CON(3),
```

```
     +                    CORR(ICORR,K1), RESULT(13), RINV(IRINV,K),
     +                    SSP(ISSP,K1), W(IW,K), XBAR(K1)
*      .. External Subroutines ..
       EXTERNAL           G02CGF
*      .. Executable Statements ..
       WRITE (NOUT,*) 'G02CGF Example Program Results'
*      Skip heading in data file
       READ (NIN,*)
       READ (NIN,*) (XBAR(I),I=1,K1), ((SSP(I,J),J=1,K1),I=1,K1),
      +  ((CORR(I,J),J=1,K1),I=1,K1)
       WRITE (NOUT,*)
       WRITE (NOUT,*) 'Means:'
       WRITE (NOUT,99999) (I,XBAR(I),I=1,K1)
       WRITE (NOUT,*)
       WRITE (NOUT,*) 'Sums of squares and cross-products about means:'
       WRITE (NOUT,99998) (J,J=1,K1)
       WRITE (NOUT,99997) (I,(SSP(I,J),J=1,K1),I=1,K1)
       WRITE (NOUT,*)
       WRITE (NOUT,*) 'Correlation coefficients:'
       WRITE (NOUT,99998) (J,J=1,K1)
       WRITE (NOUT,99997) (I,(CORR(I,J),J=1,K1),I=1,K1)
       WRITE (NOUT,*)
       IFAIL = 1
*
       CALL G02CGF(N,K1,K,XBAR,SSP,ISSP,CORR,ICORR,RESULT,COEFFT,ICOEFF,
      +            CON,RINV,IRINV,C,IC,W,IW,IFAIL)
```

```
*
      IF (IFAIL.NE.0) THEN
         WRITE (NOUT,99996) 'Routine fails, IFAIL =', IFAIL
      ELSE
         WRITE (NOUT,*) 'Vble     Coefft       Std err      t-value'
         WRITE (NOUT,99995) (I,(COEFFT(I,J),J=1,3),I=1,K)
         WRITE (NOUT,*)
         WRITE (NOUT,99994) 'Const', (CON(I),I=1,3)
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Analysis of regression table :-'
         WRITE (NOUT,*)
         WRITE (NOUT,*)
     +'      Source         Sum of squares  D.F.    Mean square      F-val
     +ue'
         WRITE (NOUT,*)
         WRITE (NOUT,99993) 'Due to regression', (RESULT(I),I=1,4)
         WRITE (NOUT,99993) 'About  regression', (RESULT(I),I=5,7)
         WRITE (NOUT,99993) 'Total             ', (RESULT(I),I=8,9)
         WRITE (NOUT,*)
         WRITE (NOUT,99992) 'Standard error of estimate =', RESULT(10)
         WRITE (NOUT,99992) 'Multiple correlation (R)   =', RESULT(11)
         WRITE (NOUT,99992) 'Determination (R squared)  =', RESULT(12)
         WRITE (NOUT,99992) 'Corrected R squared        =', RESULT(13)
         WRITE (NOUT,*)
         WRITE (NOUT,*)
     +     'Inverse of correlation matrix of independent variables:'
```

```
         WRITE (NOUT,99991) (J,J=1,K)
         WRITE (NOUT,99990) (I,(RINV(I,J),J=1,K),I=1,K)
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Modified inverse matrix:'
         WRITE (NOUT,99991) (J,J=1,K)
         WRITE (NOUT,99990) (I,(C(I,J),J=1,K),I=1,K)
      END IF
      STOP
*
99999 FORMAT (1X,I4,F16.4)
99998 FORMAT (1X,5I16)
99997 FORMAT (1X,I4,10F18.4)
99996 FORMAT (1X,A,I3)
99995 FORMAT (1X,I3,F16.9,2F16.4)
99994 FORMAT (1X,A,F11.6,2F16.4)
99993 FORMAT (1X,A,F18.4,F8.0,2F16.4)
99992 FORMAT (1X,A,F12.4)
99991 FORMAT (1X,4I10)
99990 FORMAT (1X,I4,9F10.4)
      END
```

D.5 NAG Routine E04MBF

Algorithm 5 Fortran Code for E04MBF [62]

```
*     E04MBF Example Program Text
```

```
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NCLIN, NROWA, N, NCTOTL, LIWORK, LWORK
      PARAMETER        (NCLIN=600,NROWA=NCLIN,N=7,NCTOTL=NCLIN+N,
     +                 LIWORK=2*N,LWORK=2*N*N+6*N+N+4*NCLIN+NROWA)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      DOUBLE PRECISION OBJLP
      INTEGER          I, IFAIL, ITMAX, J, MSGLVL
      LOGICAL          LINOBJ
*     .. Local Arrays ..
      DOUBLE PRECISION A(NROWA,N), BL(NCTOTL), BU(NCTOTL),
     +                 CLAMDA(NCTOTL), CVEC(N), WORK(LWORK), X(N)
      INTEGER          ISTATE(NCTOTL), IWORK(LIWORK)
*     .. External Subroutines ..
      EXTERNAL         E04MBF, X04ABF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'E04MBF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      CALL X04ABF(1,NOUT)
      ITMAX = 20
      MSGLVL = 1
      LINOBJ = .TRUE.
      READ (NIN,*) (CVEC(J),J=1,N)
```

```
      READ (NIN,*) ((A(I,J),J=1,N),I=1,NCLIN)
      READ (NIN,*) (BL(J),J=1,NCTOTL)
      READ (NIN,*) (BU(J),J=1,NCTOTL)
      READ (NIN,*) (X(J),J=1,N)
      IFAIL = 1
*
      CALL E04MBF(ITMAX,MSGLVL,N,NCLIN,NCTOTL,NROWA,A,BL,BU,CVEC,LINOBJ,
     +            X,ISTATE,OBJLP,CLAMDA,IWORK,LIWORK,WORK,LWORK,IFAIL)
*
      STOP
      END
```

D.6 Stepwise Regression Routine (RSTEP)

Algorithm 6 Fortran Code for RSTEP [49]

```
INTEGER  LDCOEF, LDCOV, LDCOVS, NVAR
PARAMETER (NVAR=10, LDCOEF=NVAR, LDCOV=NVAR, LDCOVS=NVAR)
INTEGER  IEND, INVOKE, IPRINT, ISTEP, LEVEL(NVAR), NFORCE,
     &           NOBS, NSTEP
REAL     AMACH, AOV(13), COEF(LDCOEF,5), COV(LDCOV,NVAR),
     &           COVS(LDCOVS,NVAR), HIST(NVAR), PIN, POUT,
     &    SCALE(NVAR), TOL
EXTERNAL AMACH, RSTEP
OPEN(FILE='step.in',UNIT=20)
DO I=1,NVAR
```

```
READ(20,*)(COV(I,J),J=1,NVAR)
ENDDO
DATA LEVEL/9*1, -1/
INVOKE=0
NFORCE=0
NSTEP=-1
ISTEP=0
NOBS=183
PIN=0.05
POUT=0.10
TOL=100.0*AMACH(4)
IPRINT=2
CALL RSTEP (INVOKE, NVAR, COV, LDCOV, LEVEL, NFORCE, NSTEP,
     &        ISTEP, NOBS, PIN, POUT, TOL, IPRINT, SCALE, HIST,
     &        IEND, AOV, COEF, LDCOEF, COVS, LDCOVS)
END
```

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